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INTEGRAL EQUATION METHODS FOR ELECTROSTATICS, ACOUSTICS, AND ELECTROMAGNETICS IN SMOOTHLY VARYING, ANISOTROPIC MEDIA*

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Abstract. We present a collection of well-conditioned integral equation methods for the solution of electrostatic, acoustic, or electromagnetic scattering problems involving anisotropic, inhomogeneous media. In the electromagnetic case, our approach involves a minor modification of a classical formulation. In the electrostatic or acoustic setting, we introduce a new vector partial differential equation, from which the desired solution is easily obtained. It is the vector equation for which we derive a well-conditioned integral equation. In addition to providing a unified framework for these solvers, we illustrate their performance using iterative solution methods coupled with the FFT-based technique of [F. Vico, L. Greengard, M. Ferrando, *J. Comput. Phys.*, 323 (2016), pp. 191–203] to discretize and apply the relevant integral operators.

Key words. integral equations, anisotropic media, inhomogeneous media, electrostatics, acoustics, electromagnetics

AMS subject classifications. 31B10, 35Q60, 35Q61, 45B05, 65N80, 65R20, 65Z05

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1. Introduction.

In this paper, we develop fast, high order accurate integral equation methods for several classes of elliptic partial differential equations (PDEs) in three dimensions involving anisotropic, inhomogeneous media. In the electrostatic setting, we consider the anisotropic Laplace equation

$$\nabla \cdot \epsilon(\boldsymbol{x}) \nabla \phi(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \mathbb{R}^3 \,, \tag{1.1}$$

where $\epsilon(\boldsymbol{x})$ is a real, 3×3 symmetric matrix, subject to certain regularity conditions discussed below. We also assume $\epsilon(\boldsymbol{x})$ is a compact perturbation of the identity operator I, that is, $\epsilon(\boldsymbol{x}) - I$ has compact support. A typical objective is to determine the response of the inclusion to a known, applied static field, with the response satisfying suitable decay conditions at infinity.

For acoustic or electromagnetic modeling in the frequency domain, we consider the anisotropic Helmholtz equation

$$\nabla \cdot \epsilon^{-1}(\boldsymbol{x}) \nabla \phi(\boldsymbol{x}) + \omega^2 \phi(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \mathbb{R}^3, \tag{1.2}$$

and the anisotropic Maxwell equations

$$\begin{aligned} \nabla \times \boldsymbol{E}(\boldsymbol{x}) &= i\omega\mu(\boldsymbol{x})\boldsymbol{H}(\boldsymbol{x}), \\ \nabla \times \boldsymbol{H}(\boldsymbol{x}) &= -i\omega\epsilon(\boldsymbol{x})\boldsymbol{E}(\boldsymbol{x}), \qquad \boldsymbol{x} \in \mathbb{R}^3, \end{aligned} \tag{1.3}$$

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respectively. Here, $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are complex-valued 3×3 matrices, subject to regularity and spectral properties to be discussed in detail. We again assume that $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are compact perturbations of the identity. A typical objective is to determine the response of the inclusion to an impinging acoustic or electromagnetic wave, with the response satisfying suitable radiation conditions at infinity. For a thorough discussion of the origins and applications of these problems, we refer the reader to the textbooks [9, 18, 22].

Instead of discretizing the PDEs themselves, we will develop integral representations of the solution that satisfy the outgoing decay/radiation conditions exactly, avoiding the need for truncating the computational domain and imposing approximate outgoing boundary conditions. The resulting integral equations will be shown to involve equations governed by operators of the form $I+B+K$, where I is the identity, B is a linear contraction mapping, K is compact. A simple argument based on the Neumann series allows us to extend the Fredholm alternative to this setting (and therefore to prove existence for the original, anisotropic, elliptic PDEs themselves). Moreover, our formulations permit high-order accurate discretization and FFT-based acceleration on uniform grids. In the electromagnetic case, our approach is closely related to some classical formulations. For the Laplace and Helmholtz equations, however, our approach appears to be new and depends on the construction of a *vector* PDE from which the desired solution is easily obtained. It is the vector PDE for which we will derive a new, well-conditioned integral equation. One purpose of the present paper is to describe all of these solvers in a unified framework. Given that resonance-free second kind integral equations are typically well-conditioned, they are suitable for discretization coupled with simple iterative methods such as GMRES [30] and Bi-CGStab [34] without any preconditioner. We use the method of [35] to discretize and apply the integral operators with high order accuracy and demonstrate the performance of our scheme with several numerical examples.

We will use the language of scattering theory throughout. Thus, for the scalar equations, we write $\phi = \phi^{\text{inc}} + \phi^{\text{scat}}$, where ϕ^{inc} is a known function that satisfies the homogeneous, isotropic Laplace or Helmholtz equation in free space away from sources. In the electrostatic case, ϕ^{scat} is assumed to satisfy the decay condition

$$\lim_{r\to\infty} \phi^{\text{scat}} = o(1), \tag{1.4}$$

where $r = |\boldsymbol{x}|$. In the acoustic case [10], ϕ^{scat} is assumed to satisfy the Sommerfeld radiation condition

$$\lim_{r\to\infty} r\left(\frac{\partial \phi^{\text{scat}}}{\partial r} - i\omega\phi^{\text{scat}}\right) = 0. \tag{1.5}$$

In the electromagnetic setting (1.3), we write $\boldsymbol{E} = \boldsymbol{E}^{\text{inc}} + \boldsymbol{E}^{\text{scat}}$ and $\boldsymbol{H} = \boldsymbol{H}^{\text{inc}} + \boldsymbol{H}^{\text{scat}}$, with $\boldsymbol{E}^{\text{inc}}, \boldsymbol{H}^{\text{inc}}$ corresponding to a known solution of the homogeneous, isotropic Maxwell equations in free space away from sources. $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}}$ are assumed to satisfy the Silver–Müller radiation condition [10]:

$$\lim_{r\to\infty} \left(\boldsymbol{H}^{\text{scat}} \times \boldsymbol{x} - r\boldsymbol{E}^{\text{scat}}\right) = 0. \tag{1.6}$$

2. The anisotropic Helmholtz equation. We first consider the acoustic scattering problem, and assume that the matrix $\epsilon(\boldsymbol{x})$ is a compact perturbation of the identity with entries in $C^1(\mathbb{R}^3)$. We also assume that $\epsilon(\boldsymbol{x})$ can be diagonalized in the form

$$\epsilon(\boldsymbol{x}) = U(\boldsymbol{x}) D(\boldsymbol{x}) U^*(\boldsymbol{x}),$$

where $U(\boldsymbol{x})$ is a unitary complex matrix and $D(\boldsymbol{x})$ is a diagonal matrix with positive definite real part (with entries bounded away from zero) and a positive semidefinite imaginary part (see [29]). After proving a uniqueness result, we introduce a related vector Helmholtz equation that will be used to establish existence using Fredholm theory. At the end of the section, we discuss some of the issues raised in relaxing this assumption as well as the modifications required in the zero frequency limit, leading to the electrostatic case.

DEFINITION 2.1. *By the* anisotropic Helmholtz scattering problem*, we mean the determination of a function* $\phi^{\text{scat}}(\boldsymbol{x}) \in H^1_{loc}(\mathbb{R}^3)$ *that satisfies the equation:*

$$\nabla \cdot \epsilon^{-1}(\boldsymbol{x})\nabla\phi^{\text{scat}}(\boldsymbol{x}) + \omega^2\phi^{\text{scat}}(\boldsymbol{x}) = -\nabla\cdot(\epsilon^{-1}(\boldsymbol{x}) - I)\nabla\phi^{\text{inc}}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^3, \tag{2.1}$$

where ϕ^{inc} *is a known function with*

$$\Delta\phi^{\text{inc}}(\boldsymbol{x}) + \omega^2\phi^{\text{inc}}(\boldsymbol{x}) = 0$$

in the support of $\epsilon(\boldsymbol{x}) - I$*, and* $\phi^{\text{scat}}(\boldsymbol{x})$ *must satisfy the Sommerfeld radiation condition* (1.5) *uniformly for all directions* $\frac{\boldsymbol{x}}{|\boldsymbol{x}|}$*.*

THEOREM 2.2 (uniqueness). *The anisotropic Helmholtz scattering problem has at most one solution.*

Proof. The result follows from arguments analogous to those presented in [15, section 2]. Let B_R be an open ball centered at the origin that covers the support of $\epsilon(\boldsymbol{x}) - I$. We can write (2.1) in weak form by making use of the Dirichlet-to-Neumann operator T for the exterior of the sphere $S_R = \partial B_R$:

$$\begin{aligned} &\int_{B_R} \nabla\psi(\boldsymbol{x})\cdot\epsilon^{-1}(\boldsymbol{x})\nabla\phi^{\text{scat}}(\boldsymbol{x}) - \omega^2\psi(\boldsymbol{x})\phi^{\text{scat}}(\boldsymbol{x})dV \\ &\quad = \int_{\partial B_R}\psi T[\phi^{\text{scat}}]dS - \int_{B_R}\nabla\psi(\boldsymbol{x})\cdot(\epsilon^{-1}(\boldsymbol{x}) - I)\nabla\phi^{\text{inc}}(\boldsymbol{x})dV. \end{aligned} \tag{2.2}$$

Assuming the right-hand side of (2.1) is zero we obtain

$$\int_{\partial B_R}\psi T(\phi^{\text{scat}})dS = \int_{B_R}\nabla\psi(\boldsymbol{x})\cdot\epsilon(\boldsymbol{x})^{-1}(\boldsymbol{x})\nabla\phi^{\text{scat}}(\boldsymbol{x}) - \psi(\boldsymbol{x})\omega^2\phi^{\text{scat}}(\boldsymbol{x})dV \tag{2.3}$$

for all $\psi \in H^1(B_R)$. Letting $\psi = \overline{\phi^{\text{scat}}}$ and taking complex conjugates, we have

$$\int_{\partial B_R}\phi^{\text{scat}}\frac{\partial\overline{\phi^{\text{scat}}}}{\partial n}dS = \int_{B_R}\nabla\phi^{\text{scat}}\cdot(\boldsymbol{x})\overline{\epsilon(\boldsymbol{x})^{-1}\nabla\phi^{\text{scat}}(\boldsymbol{x})} - \omega^2|\phi^{\text{scat}}(\boldsymbol{x})|^2dV, \tag{2.4}$$

so that

$$\Im\left(\int_{\partial B_R}\phi^{\text{scat}}\frac{\partial\overline{\phi^{\text{scat}}}}{\partial n}dS\right) = \Im\left(\int_{B_R}\nabla\phi^{\text{scat}}\cdot(\boldsymbol{x})\overline{\epsilon(\boldsymbol{x})^{-1}\nabla\phi^{\text{scat}}(\boldsymbol{x})}\right). \tag{2.5}$$

Moreover from our assumptions about ϵ, namely. that $\epsilon(\boldsymbol{x}) = U(\boldsymbol{x})D(\boldsymbol{x})U^*(\boldsymbol{x})$, the right-hand side can be written as

$$\nabla\phi^{\text{scat}}(\boldsymbol{x})\cdot\overline{\epsilon(\boldsymbol{x})^{-1}\nabla\phi^{\text{scat}}(\boldsymbol{x})} = \xi(\boldsymbol{x})\cdot\overline{D^{-1}(\boldsymbol{x})\xi(\boldsymbol{x})} = \sum_{i=1}^{3}|\xi_i(\boldsymbol{x})|^2\overline{D_{ii}^{-1}(\boldsymbol{x})},$$

where $\xi(\boldsymbol{x}) = U^*(\boldsymbol{x})\nabla\phi^{\text{scat}}$. Thus,

$$\Im\left(\int_{\partial B_R} \phi^{\text{scat}} \frac{\partial \overline{\phi^{\text{scat}}}}{\partial n} dS\right) \geq 0. \tag{2.6}$$

From Rellich's lemma [10], we may conclude that $\phi^{\text{scat}}(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^3/B_R$. It then follows from [13, Theorem 1 in section 6.3.1] that $\phi^{\text{scat}} \in H^2(B_R)$. As a result, (2.1) is satisfied in a strong sense and we can use the unique continuation theorem [17, Theorem 17.2.6] to conclude that $\phi^{\text{scat}}(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^3$. ∎

The essential idea underlying the derivation of a well-conditioned formulation involves recasting the scalar problem of interest in terms of a vector-valued PDE.

Definition 2.3. *By the* vector Helmholtz scattering problem *we mean the determination of a vector function* $\mathbf{F}^{\text{scat}}(\boldsymbol{x}) \in H^2_{loc}(\mathbb{R}^3)$ *satisfying the equation*

$$\Delta\mathbf{F}^{\text{scat}} + \omega^2\mathbf{F}^{\text{scat}} + (\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{scat}} = -(\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{inc}}, \tag{2.7}$$

where $\mathbf{F}^{\text{inc}}(\boldsymbol{x})$ *is a known function defined on the support of* $\epsilon(\boldsymbol{x}) - I$ *satisfying the homogeneous equation* $\Delta\boldsymbol{F}^{\text{inc}} + \omega^2\boldsymbol{F}^{\text{inc}} = 0$, *and the standard radiation condition*

$$\nabla\times\mathbf{F}^{\text{scat}}(\boldsymbol{x})\times\tfrac{\boldsymbol{x}}{|\boldsymbol{x}|} + \tfrac{\boldsymbol{x}}{|\boldsymbol{x}|}\nabla\cdot\mathbf{F}^{\text{scat}}(\boldsymbol{x}) - i\omega\mathbf{F}^{\text{scat}}(\boldsymbol{x}) = o\left(\tfrac{1}{|\boldsymbol{x}|}\right), \qquad |\boldsymbol{x}|\to\infty, \tag{2.8}$$

is satisfied uniformly in all directions $\frac{\boldsymbol{x}}{|\boldsymbol{x}|}$.

Note that in the vector Helmholtz scattering problem, the entries of ϵ^{-1} are not acted on by a differential operator. Thus, we will consider solutions of (2.7) in a strong sense, without loss of generality.

Lemma 2.4. *If* $\mathbf{F}^{\text{scat}}(\boldsymbol{x}) \in H^2_{loc}(\mathbb{R}^3)$ *satisfies the vector Helmholtz scattering problem in a strong sense, then* $\phi^{\text{scat}}(\boldsymbol{x}) := \nabla\cdot\mathbf{F}^{\text{scat}}(\boldsymbol{x}) \in H^1_{loc}(\mathbb{R}^3)$ *satisfies the anisotropic Helmholtz scattering problem in a weak sense, with the right-hand side given by the incoming field* $\phi^{\text{inc}} := \nabla\cdot\mathbf{F}^{\text{inc}}$.

Proof. Letting B_R be an open ball centered at the origin that covers the support of $\epsilon(\boldsymbol{x}) - I$, it is clear that the governing equation in the region $E = \mathbb{R}^3\backslash B_R$ is simply the isotropic, homogeneous Helmholtz equation. Thus, by standard results on the regularity of coefficients [14, Corollary 8.11], the solution $\mathbf{F}^{\text{scat}}$ is infinitely differentiable in E. We may, therefore, interpret the radiation condition in the strong sense. From the representation [10, Theorems 4.11 and 4.13] applied to the region E, we find that $\phi^{\text{scat}}(\boldsymbol{x}) := \nabla\cdot\boldsymbol{F}^{\text{scat}}(\boldsymbol{x})$ satisfies the radiation condition (1.5).

Now let $\psi \in H^1(B_R)$. From (2.7), we have

$$\nabla\psi\cdot\left(\Delta\mathbf{F}^{\text{scat}} + \omega^2\mathbf{F}^{\text{scat}} + (\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{scat}}\right) = -\nabla\psi\cdot(\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{inc}}. \tag{2.9}$$

Combined with the vector identity $\Delta\mathbf{F}^{\text{scat}} = -\nabla\times\nabla\times\mathbf{F}^{\text{scat}} + \nabla\nabla\cdot\mathbf{F}^{\text{scat}}$, this yields

$$\nabla\psi\cdot\left(-\nabla\times\nabla\times\mathbf{F}^{\text{scat}} + \omega^2\mathbf{F}^{\text{scat}} + \epsilon^{-1}\nabla\nabla\cdot\mathbf{F}^{\text{scat}}\right) = -\nabla\psi\cdot(\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{inc}}. \tag{2.10}$$

Integrating over the volume B_R and using the divergence theorem, we obtain

$$\begin{aligned}\int_{B_R} \nabla\psi\cdot\epsilon^{-1}\nabla\nabla\cdot\mathbf{F}^{\text{scat}} - \omega^2\psi\nabla\cdot\mathbf{F}^{\text{scat}} dV = &\int_{\partial B_R} \psi\boldsymbol{n}\cdot\left(\nabla\times\nabla\times\mathbf{F}^{\text{scat}} - \omega^2\mathbf{F}^{\text{scat}}\right) dV \\ &- \int_{B_R} \nabla\psi\cdot(\epsilon^{-1} - I)\nabla\nabla\cdot\mathbf{F}^{\text{inc}} dV.\end{aligned} \tag{2.11}$$

This can be rewritten in the form

$$\int_{B_R} \nabla\psi \cdot \epsilon^{-1}\nabla\nabla\cdot\mathbf{F}^{\rm scat} - \omega^2\psi\nabla\cdot\mathbf{F}^{\rm scat}dV = \int_{\partial B_R}\psi\boldsymbol{n}\cdot\Big(-\Delta\mathbf{F}^{\rm scat}-\omega^2\mathbf{F}^{\rm scat}+\nabla\nabla\cdot\mathbf{F}^{\rm scat}\Big)dV - \int_{B_R}\nabla\psi\cdot(\epsilon^{-1}-I)\nabla\nabla\cdot\mathbf{F}^{\rm inc}dV. \tag{2.12}$$

Since $\Delta\mathbf{F}^{\rm scat}(\boldsymbol{x})+\omega^2\mathbf{F}^{\rm scat}(\boldsymbol{x})=0$ for $\boldsymbol{x}\in\partial B_R$, we have the simpler equation

$$\begin{aligned}&\int_{B_R}\nabla\psi\cdot\epsilon^{-1}\nabla\nabla\cdot\mathbf{F}^{\rm scat}-\omega^2\psi\nabla\cdot\mathbf{F}^{\rm scat}dV\\ &\quad=\int_{\partial B_R}\psi T[\nabla\cdot\mathbf{F}^{\rm scat}]dS-\int_{B_R}\nabla\psi\cdot(\epsilon^{-1}-I)\nabla\nabla\cdot\mathbf{F}^{\rm inc}dV.\end{aligned}\tag{2.13}$$

It follows $\phi^{\rm scat}:=\nabla\cdot\mathbf{F}^{\rm scat}$ satisfies (2.2) for $\phi^{\rm inc}=\nabla\cdot\mathbf{F}^{\rm inc}$, the desired result. ∎

THEOREM 2.5 (uniqueness). *The Vector Helmholtz scattering problem has at most one solution.*

Proof. Let $\boldsymbol{F}^{\rm scat}\in H^2_{loc}(\mathbb{R}^3)$ be a solution of the homogeneous equation

$$\Delta\boldsymbol{F}^{\rm scat}+\omega^2\boldsymbol{F}^{\rm scat}+(\epsilon^{-1}-I)\nabla\nabla\cdot\boldsymbol{F}^{\rm scat}=0 \tag{2.14}$$

that satisfies the radiation condition. From Lemma 2.4, $\nabla\cdot\mathbf{F}^{\rm scat}$ satisfies the homogeneous equation (2.3). Theorem 2.2 then shows that $\nabla\cdot\mathbf{F}^{\rm scat}=0$. Therefore, we have that $\Delta\mathbf{F}^{\rm scat}(\boldsymbol{x})+\omega^2\mathbf{F}^{\rm scat}(\boldsymbol{x})=0$ for all $\boldsymbol{x}\in\mathbb{R}^3$, so that $\mathbf{F}^{\rm scat}=0$ for all $\boldsymbol{x}\in\mathbb{R}^3$. ∎

In order to make use of the Fredholm alternative to complete our proof of existence, we introduce the following operators:

$$\begin{aligned}&\mathcal{V}_0(\boldsymbol{J}):=\int_{\mathbb{R}^3}\frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\boldsymbol{J}(\boldsymbol{y})dV_{\boldsymbol{y}}, \quad \mathcal{V}_\omega(\boldsymbol{J}):=\int_{\mathbb{R}^3}\frac{e^{i\omega|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\boldsymbol{J}(\boldsymbol{y})dV_{\boldsymbol{y}},\\ &\mathcal{T}_0(\boldsymbol{J}):=\frac{\boldsymbol{J}}{2}+\nabla\nabla\cdot\mathcal{V}_0(\boldsymbol{J}), \qquad \mathcal{T}_\omega(\boldsymbol{J}):=\frac{\boldsymbol{J}}{2}+\nabla\nabla\cdot\mathcal{V}_\omega(\boldsymbol{J}).\end{aligned}\tag{2.15}$$

It is well known that the operator $\mathcal{T}_\omega-\mathcal{T}_0$ is compact on $L^2(\mathbb{R}^3)$ (see [11, 29]). We will also require the following two lemmas.

LEMMA 2.6. *Let H_ϵ denote the operator mapping $L^2(\mathbb{R}^3)\to L^2(\mathbb{R}^3)$ with*

$$H_\epsilon(\boldsymbol{J}):\boldsymbol{x}\mapsto\rho_\epsilon(\boldsymbol{x})\boldsymbol{J}(\boldsymbol{x}), \tag{2.16}$$

where

$$\rho_\epsilon(\boldsymbol{x}):=(\epsilon(\boldsymbol{x})+I)^{-1}(\epsilon(\boldsymbol{x})-I). \tag{2.17}$$

Then, $\|H_\epsilon\|_{L^2(\mathbb{R}^3)}<1$.

Proof. For $z\in\mathbb{C}$, let $f(z)=\frac{z-1}{z+1}$. f maps the open half-space $\Re z>0$ to $|f(z)|<1$. Since $\epsilon(\boldsymbol{x})$ is assumed to be real symmetric and uniformly elliptic, it is expressible in diagonal form as $\epsilon(\boldsymbol{x})=U(\boldsymbol{x})D(\boldsymbol{x})U^*(\boldsymbol{x})$, with the diagonal elements of $D(\boldsymbol{x})$ positive and bounded away from zero [13]. It follows that $\rho_\epsilon(\boldsymbol{x})=U(\boldsymbol{x})f(D)(\boldsymbol{x})U^*(\boldsymbol{x})\in L^\infty(\mathbb{R}^3)$, with eigenvalues strictly bounded by one, proving the desired result. ∎

LEMMA 2.7. *The operator $2\mathcal{T}_0$ is an isometry on $L^2(\mathbb{R}^3)$. That is, $\|2\mathcal{T}_0\|_{L^2(\mathbb{R}^3)} = 1$.*

Proof. Using the Helmholtz decomposition (see, for example, [8, Theorem 14]), we can write $\boldsymbol{J} = \nabla\psi + \nabla \times \mathbf{P}$. It is straightforward to check that $2\mathcal{T}_0(\nabla \times \mathbf{P}) = \nabla \times \mathbf{P}$, while $2\mathcal{T}_0(\nabla\phi) = -\nabla\phi$. Thus, $2\mathcal{T}_0(\boldsymbol{J}) = -\nabla\psi + \nabla \times \mathbf{P}$ and the result follows immediately from the orthogonality of the Helmholtz decomposition. ∎

THEOREM 2.8 (existence). *The anisotropic scalar and vector Helmholtz scattering problems have solutions.*

Proof. Note first that the vector field $\boldsymbol{F} := \mathcal{V}_\omega(\boldsymbol{J})$ is a solution of (2.7) if and only if

$$-\boldsymbol{J} + (\epsilon^{-1} - I)\nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{J}) = -(\epsilon^{-1} - I)\nabla\nabla \cdot \boldsymbol{F}^{\text{inc}}. \tag{2.18}$$

Adding and substracting $\boldsymbol{J}/2$, this is equivalent to

$$-\boldsymbol{J} + (\epsilon^{-1} - I)\left(-\frac{\boldsymbol{J}}{2} + \mathcal{T}_\omega(\boldsymbol{J})\right) = -(\epsilon^{-1} - I)\nabla\nabla \cdot \boldsymbol{F}^{\text{inc}}. \tag{2.19}$$

Multiplying by $-2(\epsilon^{-1} + I)^{-1}$ we have

$$\boldsymbol{J} + 2H_\epsilon\mathcal{T}_0(\boldsymbol{J}) + 2H_\epsilon(\mathcal{T}_\omega - \mathcal{T}_0)(\boldsymbol{J}) = -2H_\epsilon\nabla\nabla \cdot \boldsymbol{F}^{\text{inc}}, \tag{2.20}$$

where H_ϵ is defined in (2.16), where we have used the fact that $H_{\epsilon^{-1}} = -H_\epsilon$. Using Lemmas 2.6 and 2.7, we observe that the left-hand side of the resulting integral equation (2.20) is of the form $(I + B + K)\boldsymbol{J}$, where $I + B + K : L^2(B_R) \to L^2(B_R)$ with $B(\boldsymbol{J}) = 2H_\epsilon\mathcal{T}_0(\boldsymbol{J})$, $\|B\|_{L^2(B_R)} < 1$, and K compact. Since $I + B$ is invertible, we can apply Fredholm theory directly.

Uniqueness for (2.20) follows from Theorem 2.5 and the uniqueness of the representation $\boldsymbol{F} = \mathcal{V}_\omega(\boldsymbol{J})$. It is shown in [11] that the operator $\mathcal{V}_\omega$ maps $L^2(B_R)$ to $H^2(B_R)$, so that $\mathbf{F}^{\text{scat}} := \mathcal{V}_\omega(\boldsymbol{J}) \in H^2_{loc}(\mathbb{R}^3)$ for all $\boldsymbol{J} \in L^2(B_R)$. If, moreover, $\boldsymbol{J}$ satisfies (2.20), then by construction $\mathbf{F}^{\text{scat}}$ satisfies (2.7), and $\nabla \cdot \mathbf{F}^{\text{scat}} \in H^1_{loc}(\mathbb{R}^3)$ satisfies (2.3). ∎

To summarize: by solving the integral equation

$$\Big(I + 2H_\epsilon\mathcal{T}_0 + 2H_\epsilon(\mathcal{T}_\omega - \mathcal{T}_0)\Big)\boldsymbol{J} = -2H_\epsilon\nabla\phi^{\text{inc}}, \tag{2.21}$$

we obtain a solution to the vector Helmholtz scattering problem of the form $\mathbf{F}^{\text{scat}} = \mathcal{V}_\omega(\boldsymbol{J})$. The function $\phi^{\text{scat}} := \nabla \cdot \mathbf{F}^{\text{scat}}$ provides a solution to the corresponding anisotropic Helmholtz scattering problem. (The same result holds in 2 dimensions as well.)

Remark 1 (smoothness of the coefficients). In this section, we have assumed coefficients $\epsilon_{ij}(\boldsymbol{x}) \in C^1(\mathbb{R}^3)$, in order to be able to apply the unique continuation property. This regularity condition can be relaxed in various ways and the unique continuation property still holds. There is a vast literature on this subject for second order elliptic PDEs (see [19] for a good summary), following the early work of Carleman [7] and Müller [25]. While it is known that $\epsilon_{ij}(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$ is too large a class of coefficients (due to counterexamples [20, 24, 27]), there has been a lot of effort at establishing more general results [4, 5, 21, 31]. The class of coefficients which are piecewise smooth where the jumps occur on C^2 boundaries was studied in [15]. In [6], piecewise homogeneous objects were studied. It would be of great practical interest if the unique continuation property holds for piecewise smooth coefficients, whose jumps occur on piecewise C^2 boundaries, allowing our integral formulation to be applicable to domains with edges. This would follow naturally, since the existence theorem (Theorem 2.8) only requires $\epsilon_{ij}(\boldsymbol{x}) \in L^\infty(\mathbb{R}^3)$ and a uniqueness result for the anisotropic Helmholtz scattering problem.

Remark 2 (the anisotropic Laplace equation). All of the results obtained in this section apply in the zero frequency limit, where the governing equation is the anisotropic Laplace equation $\nabla \cdot \epsilon(\boldsymbol{x})\nabla\phi^{\text{scat}}(\boldsymbol{x}) = -\nabla \cdot (\epsilon(\boldsymbol{x}) - I)\nabla\phi^{\text{inc}}(\boldsymbol{x})$. The principal difference is that the real symmetric, positive definite matrix $\epsilon(\boldsymbol{x})$ need only have bounded entries. Uniqueness can be proven using the Dirichlet-to-Neumann map on the ball B_R that contains the support of $\epsilon(\boldsymbol{x}) - I$, combined with Dirichlet's principle, rather than the Rellich lemma. Existence can be established, as above, by reformulating the problem as a vector Fredholm equation of the second kind. Since $\omega = 0$, it takes the simpler form

$$(I - 2H_\epsilon \mathcal{T}_0)\boldsymbol{J} = 2H_\epsilon \nabla\phi^{\text{inc}}, \tag{2.22}$$

rather than (2.21).

Remark 3. From a practical viewpoint, the integral equations (2.22) and (2.21) can be discretized using a Nyström method and solved iteratively to obtain a numerical solution of the original scalar problem. It is worth noting that no estimate involving derivatives of $\epsilon_{ij}(\boldsymbol{x})$ are required. Because they are Fredholm equations of the second kind, the order of accuracy obtained in the solution is the same as the order of accuracy used in the underlying quadrature rule [3]. Of course, if there are jumps in $\epsilon(\boldsymbol{x})$, then adaptive discretization methods are recommended for resolution, but additional unknowns and surface integral operators are not required to account for the effect of these discontinuities.

3. The anisotropic Maxwell's equations.

In this section we assume that $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are real, symmetric 3×3 matrices, uniformly positive definite with entries $\epsilon_{ij}(\boldsymbol{x}), \mu_{ij}(\boldsymbol{x}) \in C^2(\mathbb{R}^3)$. We also assume that $\epsilon(\boldsymbol{x}) - I$ and $\mu(\boldsymbol{x}) - I$ have compact support, where I is the 3×3 identity matrix.

DEFINITION 3.1. *By the anisotropic Maxwell scattering problem, we mean the determination of functions* $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}} \in H_{loc}(curl, \mathbb{R}^3)$ *(see* [8] *for further details) such that*

$$\begin{aligned} \nabla \times \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) - i\omega\mu(\boldsymbol{x})\boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) &= +i\omega(\mu(\boldsymbol{x}) - I)\boldsymbol{H}^{\text{inc}}(\boldsymbol{x}), \\ \nabla \times \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) + i\omega\epsilon(\boldsymbol{x})\boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) &= -i\omega(\epsilon(\boldsymbol{x}) - I)\boldsymbol{E}^{\text{inc}}(\boldsymbol{x}), \end{aligned} \tag{3.1}$$

where the incoming field $\boldsymbol{E}^{\text{inc}}, \boldsymbol{H}^{\text{inc}}$ *satisfy the free space Maxwell's equations with* $\epsilon(\boldsymbol{x}) = I, \mu(\boldsymbol{x}) = I$, *and the radiation condition,*

$$\boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) \times \frac{\boldsymbol{x}}{|\boldsymbol{x}|} - \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) = o\left(\frac{1}{|\boldsymbol{x}|}\right) \quad \text{as } |\boldsymbol{x}| \to \infty, \tag{3.2}$$

is satisfied uniformly in all directions $\frac{\boldsymbol{x}}{|\boldsymbol{x}|}$.

THEOREM 3.2 (uniqueness). *The anisotropic Maxwell scattering problem has at most one solution.*

Proof. The proof is standard and based on the Rellich lemma [11]. Assume the right-hand side of (3.1) is zero. Taking a ball B_R that contains the support of $\epsilon(\boldsymbol{x}) - I$

and $\mu(\boldsymbol{x}) - I$, we have

(3.3)
$$\Re\left(\int_{\partial B_R} \boldsymbol{n} \times \boldsymbol{E}^{\text{scat}} \cdot \overline{\boldsymbol{H}}^{\text{scat}} dS\right) = \Re\left(i\omega \int_{B_R} \overline{\boldsymbol{H}}^{\text{scat}} \cdot \mu \boldsymbol{H}^{\text{scat}} + \boldsymbol{E}^{\text{scat}} \cdot \overline{\epsilon}\overline{\boldsymbol{E}}^{\text{scat}} dV\right) = 0.$$

Since $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}}$ are analytic in $\mathbb{R}^3/B_R$, we have that $\boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) = \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^3/B_R$. Using the unique continuation property [23], we obtain $\boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) = \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \mathbb{R}^3$. ◻

In order to establish existence, we extend the technique described earlier.

THEOREM 3.3 (existence). *The anisotropic Maxwell scattering problem has a solution.*

Proof. We begin by rewriting the anisotropic Maxwell scattering problem in a manner such that the variable coefficient terms only appear in the right-hand side:

$$\begin{aligned} \nabla \times \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) - i\omega \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) &= +i\omega(\mu(\boldsymbol{x}) - I)\left(\boldsymbol{H}^{\text{inc}}(\boldsymbol{x}) + \boldsymbol{H}^{\text{scat}}(\boldsymbol{x})\right), \\ \nabla \times \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) + i\omega \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) &= -i\omega(\epsilon(\boldsymbol{x}) - I)\left(\boldsymbol{E}^{\text{inc}}(\boldsymbol{x}) + \boldsymbol{E}^{\text{scat}}(\boldsymbol{x})\right). \end{aligned} \tag{3.4}$$

We now define the right-hand sides as volume (polarization) currents:

$$\begin{aligned} \boldsymbol{J}_V(\boldsymbol{x}) &:= -i\omega(\epsilon(\boldsymbol{x}) - I)\left(\boldsymbol{E}^{\text{inc}}(\boldsymbol{x}) + \boldsymbol{E}^{\text{scat}}(\boldsymbol{x})\right), \\ \boldsymbol{M}_V(\boldsymbol{x}) &:= -i\omega(\mu(\boldsymbol{x}) - I)\left(\boldsymbol{H}^{\text{inc}}(\boldsymbol{x}) + \boldsymbol{H}^{\text{scat}}(\boldsymbol{x})\right). \end{aligned} \tag{3.5}$$

Assume now that $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}} \in C^1(\mathbb{R}^3)$ and that they satisfy the constant coefficient Maxwell system:

$$\begin{aligned} \nabla \times \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) - i\omega \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) &= -\boldsymbol{M}_V(\boldsymbol{x}), \\ \nabla \times \boldsymbol{H}^{\text{scat}}(\boldsymbol{x}) + i\omega \boldsymbol{E}^{\text{scat}}(\boldsymbol{x}) &= \boldsymbol{J}_V(\boldsymbol{x}). \end{aligned} \tag{3.6}$$

Then, applying the Stratton–Chu formulas [11, eq. 6.5], the following representation formula holds:

$$\begin{pmatrix} \boldsymbol{E}^{\text{scat}} \\ \boldsymbol{H}^{\text{scat}} \end{pmatrix} = \begin{pmatrix} \frac{-1}{i\omega}(\nabla\nabla \cdot +\omega^2)\mathcal{V}_\omega & -\nabla \times \mathcal{V}_\omega \\ \nabla \times \mathcal{V}_\omega & \frac{-1}{i\omega}(\nabla\nabla \cdot +\omega^2)\mathcal{V}_\omega \end{pmatrix} \begin{pmatrix} \boldsymbol{J}_V \\ \boldsymbol{M}_V \end{pmatrix}. \tag{3.7}$$

Conversely, if $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}}, \boldsymbol{J}_V, \boldsymbol{M}_V$ satisfy (3.7), then it is a straightforward computation to show that they satisfy (3.6). Assuming that $\boldsymbol{J}_V, \boldsymbol{M}_V$ are defined by (3.5), it is then immediate to see that $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}}$ satisfy (3.4), and equivalently (3.1). Thus, we have proven that the PDE system with inhomogeneous coefficients (3.1) is equivalent to the integral formulation (3.5)–(3.7). It is also easy to show that the equivalence holds true for fields in $H_{loc}(curl, \mathbb{R}^3)$.

Eliminating $\boldsymbol{E}^{\text{scat}}, \boldsymbol{H}^{\text{scat}}$ from (3.5)–(3.7), we obtain the following integral equation:

$$\begin{aligned} \boldsymbol{J} - H_\epsilon 2\mathcal{T}_\omega(\boldsymbol{J}) - 2H_\epsilon\omega^2\mathcal{V}_\omega(\boldsymbol{J}) - i\omega 2H_\epsilon \nabla \times \mathcal{V}_\omega(\boldsymbol{M}) &= 2H_\epsilon \boldsymbol{E}^{\text{inc}}, \\ \boldsymbol{M} - H_\mu 2\mathcal{T}_\omega(\boldsymbol{M}) - 2H_\mu\omega^2\mathcal{V}_\omega(\boldsymbol{M}) + i\omega 2H_\mu \nabla \times \mathcal{V}_\omega(\boldsymbol{J}) &= 2H_\mu \boldsymbol{H}^{\text{inc}}, \end{aligned} \tag{3.8}$$

where H_ϵ is defined in (2.16) and $H_\mu(\boldsymbol{x}) := (\mu(\boldsymbol{x}) + I)^{-1}(\mu(\boldsymbol{x}) - I)$. We also make the change of variables

$$\boldsymbol{J} := \frac{\boldsymbol{J}_V}{-i\omega}, \qquad \boldsymbol{M} := \frac{\boldsymbol{M}_V}{-i\omega}, \tag{3.9}$$

to avoid low frequency breakdown (that is, instability of the representation as $\omega \to 0$).

Using an approach similar to that in previous sections (in the function space $L^2(B_R) \times L^2(B_R)$), we can write (3.8) in the form

$$\left(I + C + K\right) \begin{pmatrix} \boldsymbol{J} \\ \boldsymbol{M} \end{pmatrix} = \begin{pmatrix} 2H_\epsilon \boldsymbol{E}^{\rm inc} \\ 2H_\mu \boldsymbol{H}^{\rm inc} \end{pmatrix},$$

where C is a contraction and K is compact. We now use the standard representation for electromagnetic fields in terms of electric and magnetic currents:

$$\begin{aligned} \boldsymbol{E}^{\rm scat} &= \nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{J}) + \omega^2 \mathcal{V}_\omega(\boldsymbol{J}) + i\omega \nabla \times \mathcal{V}_\omega(\boldsymbol{M}), \\ \boldsymbol{H}^{\rm scat} &= \nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{M}) + \omega^2 \mathcal{V}_\omega(\boldsymbol{M}) - i\omega \nabla \times \mathcal{V}_\omega(\boldsymbol{J}). \end{aligned} \tag{3.10}$$

Since the operators involved in (3.10) map $L^2(B_R)$ into $H_{loc}(curl, \mathbb{R}^3)$, uniqueness of the anisotropic Maxwell scattering problem implies uniqueness and, hence, existence for the integral equation (3.8). Finally, this yields existence for the anisotropic Maxwell scattering problem itself. ∎

To summarize, solving the integral system

$$\begin{aligned} \boldsymbol{J} - H_\epsilon 2\mathcal{T}_\omega(\boldsymbol{J}) - 2H_\epsilon \omega^2 \mathcal{V}_\omega(\boldsymbol{J}) - i\omega 2H_\epsilon \nabla \times \mathcal{V}_\omega(\boldsymbol{M}) &= 2H_\epsilon \boldsymbol{E}^{\rm inc}, \\ \boldsymbol{M} - H_\mu 2\mathcal{T}_\omega(\boldsymbol{M}) - 2H_\mu \omega^2 \mathcal{V}_\omega(\boldsymbol{M}) + i\omega 2H_\mu \nabla \times \mathcal{V}_\omega(\boldsymbol{J}) &= 2H_\mu \boldsymbol{H}^{\rm inc}, \end{aligned} \tag{3.11}$$

and computing

$$\begin{aligned} \boldsymbol{E}^{\rm scat} &= \nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{J}) + \omega^2 \mathcal{V}_\omega(\boldsymbol{J}) + i\omega \nabla \times \mathcal{V}_\omega(\boldsymbol{M}), \\ \boldsymbol{H}^{\rm scat} &= \nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{M}) + \omega^2 \mathcal{V}_\omega(\boldsymbol{M}) - i\omega \nabla \times \mathcal{V}_\omega(\boldsymbol{J}), \end{aligned} \tag{3.12}$$

provides a solution to the anisotropic Maxwell scattering problem.

For the particular case $\mu = I$, we have the following, simpler integral equation:

$$\boldsymbol{J} - H_\epsilon 2\mathcal{T}_\omega(\boldsymbol{J}) - 2H_\epsilon \omega^2 \mathcal{V}_\omega(\boldsymbol{J}) = 2H_\epsilon \boldsymbol{E}^{\rm inc}, \tag{3.13}$$

and the corresponding representation

$$\begin{aligned} \boldsymbol{E}^{\rm scat} &= \nabla\nabla \cdot \mathcal{V}_\omega(\boldsymbol{J}) + \omega^2 \mathcal{V}_\omega(\boldsymbol{J}), \\ \boldsymbol{H}^{\rm scat} &= -i\omega \nabla \times \mathcal{V}_\omega(\boldsymbol{J}). \end{aligned} \tag{3.14}$$

A closely related integral formulation (using a slightly different scaling) is widely used [33, 37, 32], and known as the "JM" volume integral formulation.

Remark 4 (nonsmooth coefficients and lossy materials). The unique continuation property for the Maxwell system (3.1) has been extended to the case $\epsilon_{ij}(\boldsymbol{x}), \mu_{ij}(\boldsymbol{x}) \in C^1(\mathbb{R}^3)$ in [12] and to the case of Lipschitz coefficients $\epsilon_{ij}(\boldsymbol{x}), \mu_{ij}(\boldsymbol{x}) \in W^{1,\infty}(B_R)$ in [26, 36]. In both settings, $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are assumed to be real (no dissipation).

Lossy materials for which the unique continuation property has been shown to hold [28] include the case when $\mu(\boldsymbol{x}) = I$ and $\epsilon(\boldsymbol{x})$ has entries $\epsilon_{ij}(\boldsymbol{x}) \in C^3(\mathbb{R}^3)$ with $\epsilon(\boldsymbol{x}) = U_1(\boldsymbol{x})D_\epsilon(\boldsymbol{x})U_1^*(\boldsymbol{x})$, where $U_1(\boldsymbol{x})$ is a unitary complex matrix and $D_\epsilon(\boldsymbol{x})$ is diagonal with diagonal entries whose real parts are positive and bounded away from zero and whose imaginary parts are nonnegative.

Note that in the proof of existence described in the previous theorem, $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are assumed to be real symmetric, with entries in $C^2(\mathbb{R}^3)$. Assuming the unique continuation property holds, extension to the complex dissipative case where both matrices $\epsilon(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ have L^∞ entries is straightforward. By this, we mean that $\epsilon(\boldsymbol{x}) = U_1(\boldsymbol{x})D_\epsilon(\boldsymbol{x})U_1^*(\boldsymbol{x})$, $\mu(\boldsymbol{x}) = U_2(\boldsymbol{x})D_\mu(\boldsymbol{x})U_2^*(\boldsymbol{x})$, where D_ϵ and D_μ have diagonal entries with strictly positive real part and nonnegative imaginary part. For further discussion, see [1, 2, 16].

4. Numerical results. We illustrate the performance of our approach by solving the integral equations (2.21) and (3.13). We begin with a uniform $n \times n \times n$ mesh on which we discretize the incoming field, the material properties, and the unknown solution vectors $\boldsymbol{J}$ and/or $\boldsymbol{M}$. We apply the various integral operators that arise using Fourier methods, as described in [35]. Very briefly, the method proceeds by (a) truncating the governing free-space Green's function (limited to the user-specified range over which we seek the solution), (b) transforming the truncated kernel—yielding a smooth function in Fourier space, and (c) imposing a high frequency cutoff defined by the grid spacing of the resolving mesh. Assuming that the data are well-resolved on this mesh, the method achieves high-order (superalgebraic) convergence. The linear systems are solved iteratively, using Bi-CGStab [34].

For the sake of simplicity, we let $\mu(\boldsymbol{x}) = I$ and study the influence of ϵ on the behavior of the numerical method. There are three parameters to consider. First is the *contrast*, defined as the maximum ratio between the eigenvalues of ϵ and the background dielectric constant. Second is the level of anisotropy, determined by the ratio of the eigenvalues of ϵ (as well as rotations of ϵ to nondiagonal form).

We assume that the computational domain is set to $[0,1]^3$. We define a bump function

$$W(x,y,z) = e^{-\left(\frac{x-0.5}{0.25}\right)^8} e^{-\left(\frac{y-0.5}{0.25}\right)^8} e^{-\left(\frac{z-0.5}{0.25}\right)^8}$$

which has decayed to zero at the edge of the computational domain to machine precision.

4.1. Isotropic scattering from a highly oscillatory structure. In our first example, we consider the interaction of an electromagnetic wave $\boldsymbol{E}^{\mathrm{inc}} = (0,0,\exp(i\omega x))$ with a highly oscillatory but locally isotropic permittivity:

$$\epsilon(x,y,z) = \Big(1 + W(x,y,z)\big(1 + .1\sin(\omega x)\sin(\omega y)\sin(\omega z)\big)\Big)I, \tag{4.1}$$

where I is the 3×3 identity matrix and $\omega = 408$. Note that the contrast is approximately 2 and that the magnitude of the oscillation is relatively small: 10% of the magnitude of the bump function $W(x,y,z)$ itself. Nevertheless, resolving ϵ at 2 points per wavelength requires at least 200 points in each component direction. We plot the z component of the scattered field $\boldsymbol{E}^{\mathrm{scat}}$ in Figure 1 after solving the integral equation (3.13).

Since we do not have an exact solution for this problem, we carry out a numerical convergence study, using a $326 \times 326 \times 326$ grid followed by a $650 \times 650 \times 650$ grid, suggesting that six digits of accuracy have been achieved on the coarser grid in both

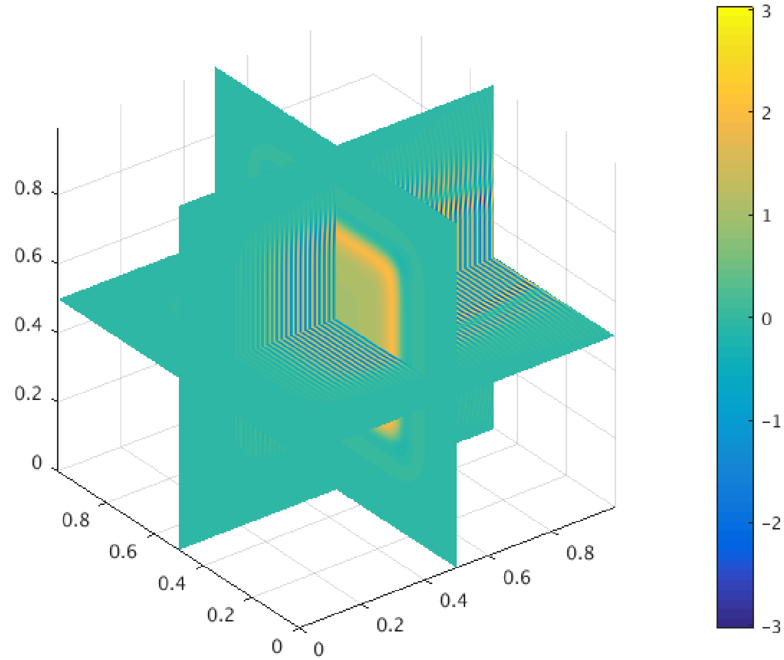

FIG. 1. *The z-component of the electric field, when solving the Maxwell scattering problem* (3.1) *with* $\omega = 408$, $\mu = I$, *and* ϵ *defined in* (4.1). *The solution is obtained from the representation* (3.14) *and the corresponding integral equation* (3.13), *discretized with* 650^3 *points.*

the L_2 and L_∞ norms. The calculation required 61 matrix-vector multiplies and 152 minutes on an Intel Xeon 2.5 GHz workstation with 60 cores and 1.5 terabytes of memory.

4.2. Strong isotropic and anisotropic scattering. To study the behavior of our integral equation formulation at higher contrast over a range of frequencies, we consider two additional locally isotropic examples and two anisotropic ones. For the isotropic cases, we let

$$\epsilon_{222}(x, y, z) := \big(1 + W(x, y, z)\big)I, \qquad \epsilon_{444}(x, y, z) = \big(1 + 3W(x, y, z)\big)I.$$

Note that ϵ_{222} has a maximum contrast of 2, while ϵ_{444} has a maximum contrast of 4. For the anisotropic examples, we let

$$\epsilon_{234}(x, y, z) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \text{ with } \begin{cases} \epsilon_1(x, y, z) = 1 + W(x, y, z), \\ \epsilon_2(x, y, z) = 1 + 2W(x, y, z), \\ \epsilon_3(x, y, z) = 1 + 3W(x, y, z), \end{cases} \tag{4.2}$$

and

$$\epsilon_{dense}(x, y, z) = R_2(\phi)R_1(\theta) \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} R_1(\theta)' R_2(\phi)', \tag{4.3}$$

where ϵ_1, ϵ_2, ϵ_3 are defined in (4.2), and the rotation matrices R_1 and R_2 are given

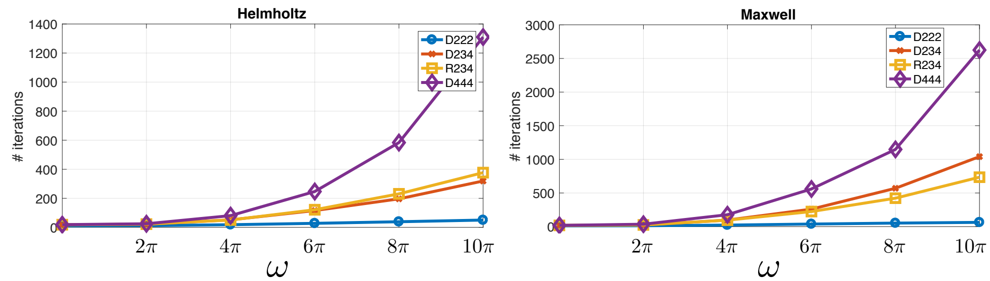

FIG. 2. *Number of iterations for convergence of Bi-CGStab with a tolerance of* 10^{-14}*, as a function of the frequency* ω *when applied to the Helmholtz integral equation* (2.21) *(left) and the Maxwell integral equation* (3.13) *(right). The labels D222, D234, R234, and D444 correspond to* ϵ_{222}*,* ϵ_{234}*,* ϵ_{dense}*, and* ϵ_{444}*, respectively.*

by

$$(4.4) \quad R_1(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix}, \quad R_2(\phi) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with $\phi(x, y, z) = \pi x$ and $\theta(x, y, z) = \pi y$.

We first examine the performance of Bi-CGStab, plotting the number of iterations required to achieve a tolerance of 10^{-14} as a function of the frequency ω for both the Helmholtz and Maxwell scattering problems on a $150 \times 150 \times 150$ grid (Figure 2). As expected, the number of iterations increases with frequency. Moreover, for a fixed frequency, the number of iterations increases with the contrast. Note, however, that the anisotropy and rotation have only limited impact on the number of iterations. Clearly, while the method is robust at low frequencies, these calculations remain challenging in strong scattering regimes.

Additional details regarding numerical experiments are provided in Tables 1–4. Note that the number of iterations is more or less constant for each fixed problem as the mesh is refined (consistent with the expected behavior of a second kind Fredholm equation). Note also that the number of iterations for the diagonally anisotropic case ϵ_{234} (Table 2) is about the same as for the case ϵ_{dense}, where the principal axes have been rotated throughout the domain (Table 3). A slice of the z-component of the electric field for the case ϵ_{Dense} is shown in Figure 3.

In the example ϵ_{444}, the number of iterations is significantly worse than in any of the other cases, even though it is locally isotropic. Thus, the behavior of the proposed integral equation (3.13) appears to be controlled by the contrast and frequency more than by anisotropy. The scatterer is approximately $(\frac{\omega}{2\pi}\sqrt{4})^3$ cubic wavelengths in size—on the order of 1000 for the largest value of ω. Thus, it is not surprising that Bi-CGStab requires many iterations to converge.

5. Discussion. We have presented a collection of Fredholm integral equations for electrostatic, acoustic, and electromagnetic scattering problems in anisotropic, inhomogeneous media. In the acoustic and electrostatic cases, our approach appears to be new, and involves recasting the scalar problem of interest in terms of a vector unknown. We have shown that high-order accuracy can be achieved using the trun-

TABLE 1

Summary of numerical results for the locally isotropic permittivity tensor ϵ_{222}. The size is defined to be the number of wavelengths of the incoming field across the unit box supporting the perturbation ϵ, namely, $\frac{\omega}{2\pi}$. N_{tot} denotes the total number of unknowns, n_{side} denotes the number of points in each linear dimension, E_2 denotes the L_2 error, E_∞ denotes the L_∞ error, N_{matvec} denotes the number of matrix-vector multiplies required, and time denotes the total time required for the computation in seconds.

Size $\left(\frac{\omega}{2\pi}\right)$	N_{tot}	n_{side}	E_2	E_∞	N_{matvec}	$Time\ (s)$
10^{-50}	$1.03\,10^6$	70	1.5×10^{-7}	1.1×10^{-6}	22	6.4
10^{-50}	$5.18\,10^6$	120	1.2×10^{-11}	7.8×10^{-11}	22	27.7
10^{-50}	$1.75\,10^7$	180	1.6×10^{-16}	1.0×10^{-15}	22	93.6
10^{-10}	$1.03\,10^6$	70	1.5×10^{-7}	1.1×10^{-6}	22	6.6
10^{-10}	$5.18\,10^6$	120	1.2×10^{-11}	7.8×10^{-11}	22	27.5
10^{-10}	$1.75\,10^7$	180	1.6×10^{-16}	1.0×10^{-15}	22	91.9
1	$1.03\,10^6$	70	1.5×10^{-7}	8.2×10^{-7}	27	8.1
1	$5.18\,10^6$	120	1.1×10^{-11}	6.0×10^{-11}	27	33.3
1	$1.75\,10^7$	180	2.4×10^{-16}	8.6×10^{-16}	27	110.1
20	$1.03\,10^6$	70	7.3×10^{-4}	1.1×10^{-3}	469	134.1
20	$5.18\,10^6$	120	4.9×10^{-10}	1.2×10^{-9}	426	487.5
20	$1.75\,10^7$	180	1.9×10^{-14}	1.8×10^{-14}	426	1614.8

TABLE 2

Summary of numerical results for the anisotropic permittivity tensor ϵ_{234}. See Table 1 for an explanation of the column headers.

Size $\left(\frac{\omega}{2\pi}\right)$	N_{tot}	n_{side}	E_2	E_∞	N_{matvec}	$Time\ (s)$
10^{-50}	$1.03\,10^6$	70	3.1×10^{-6}	1.9×10^{-5}	37	10.9
10^{-50}	$5.18\,10^6$	120	1.7×10^{-9}	8.5×10^{-9}	37	44.9
10^{-50}	$1.75\,10^7$	180	1.7×10^{-13}	9.9×10^{-13}	37	148.8
10^{-10}	$1.03\,10^6$	70	3.1×10^{-6}	1.9×10^{-5}	37	10.8
10^{-10}	$5.18\,10^6$	120	1.7×10^{-9}	8.5×10^{-9}	37	45.4
10^{-10}	$1.75\,10^7$	180	1.7×10^{-13}	9.9×10^{-13}	37	148.5
1	$1.03\,10^6$	70	2.2×10^{-6}	1.0×10^{-5}	48	14.4
1	$5.18\,10^6$	120	1.2×10^{-9}	4.3×10^{-9}	48	57.2
1	$1.75\,10^7$	180	1.2×10^{-13}	6.4×10^{-13}	50	198.1
5	$1.03\,10^6$	70	1.8×10^{-6}	7.7×10^{-6}	2125	611.8
5	$5.18\,10^6$	120	9.6×10^{-10}	3.0×10^{-9}	2081	2378.1
5	$1.75\,10^7$	180	8.9×10^{-14}	3.6×10^{-13}	2105	7948.1

cated kernel method of [35] and the FFT. We have also shown that problems with low or moderate contrast are rapidly solved using the Bi-CGStab iterative method, even with nearly one billion unknowns on a single multicore workstation. Once the domain is many wavelengths in size, however, and the contrast is large, we have found that both Bi-CGStab and GMRES perform rather poorly. In our largest high-contrast example, the scatterer is approximately 1000 cubic wavelengths in size, and it is not surprising that multiple interior scattering events cause difficulties. This suggests two avenues for further research: either the development of fast, direct solvers (for which

TABLE 3
Summary of numerical results for the anisotropic permittivity tensor ϵ_{dense}. See Table 1 for an explanation of the column headers.

Size $\left(\frac{\omega}{2\pi}\right)$	N_{tot}	n_{side}	E_2	E_∞	N_{matvec}	$Time\ (s)$
10^{-50}	$1.03\,10^6$	70	1.3×10^{-6}	7.7×10^{-6}	37	10.6
10^{-50}	$5.18\,10^6$	120	4.1×10^{-10}	1.8×10^{-9}	37	45.3
10^{-50}	$1.75\,10^7$	180	2.0×10^{-14}	1.6×10^{-13}	37	149.2
10^{-10}	$1.03\,10^6$	70	1.3×10^{-6}	7.7×10^{-6}	37	10.8
10^{-10}	$5.18\,10^6$	120	4.1×10^{-10}	1.8×10^{-9}	37	45.2
10^{-10}	$1.75\,10^7$	180	2.0×10^{-14}	1.6×10^{-13}	37	147.9
1	$1.03\,10^6$	70	1.3×10^{-6}	6.9×10^{-6}	50	14.7
1	$5.18\,10^6$	120	4.1×10^{-10}	2.6×10^{-9}	51	61.0
1	$1.75\,10^7$	180	1.9×10^{-14}	1.1×10^{-13}	51	202.0
5	1029000	70	1.7×10^{-6}	1.1×10^{-5}	1447	412.6
5	$5.18\,10^6$	120	5.1×10^{-10}	2.9×10^{-9}	1474	1697.6
5	$1.75\,10^7$	180	1.3×10^{-13}	2.3×10^{-13}	1478	5687.2

TABLE 4
Summary of numerical results for the locally isotropic permittivity tensor ϵ_{444}. See Table 1 for an explanation of the column headers.

Size $\left(\frac{\omega}{2\pi}\right)$	N_{tot}	n_{side}	E_2	E_∞	N_{matvec}	$Time\ (s)$
10^{-50}	$3.75\,10^5$	50	8.4×10^{-5}	4.5×10^{-4}	37	5.0
10^{-50}	$3.00\,10^6$	100	3.8×10^{-8}	2.1×10^{-7}	38	27.9
10^{-50}	$1.01\,10^7$	150	1.5×10^{-11}	9.3×10^{-11}	38	87.7
10^{-50}	$3.19\,10^7$	220	8.5×10^{-15}	1.5×10^{-14}	38	271.9
10^{-10}	$3.75\,10^5$	50	8.4×10^{-5}	4.5×10^{-4}	37	5.1
10^{-10}	$3.00\,10^6$	100	3.8×10^{-8}	2.1×10^{-7}	38	27.9
10^{-10}	$1.01\,10^7$	150	1.5×10^{-11}	9.3×10^{-11}	38	88.7
10^{-10}	$3.19\,10^7$	220	8.6×10^{-15}	1.5×10^{-14}	38	273.9
1	$3.75\,10^5$	50	6.9×10^{-5}	2.5×10^{-4}	61	7.9
1	$3.00\,10^6$	100	3.1×10^{-8}	1.3×10^{-7}	69	49.5
1	$1.01\,10^7$	150	1.2×10^{-11}	4.5×10^{-11}	72	161.5
1	$3.19\,10^7$	220	1.6×10^{-13}	1.7×10^{-13}	68	472.3
5	$3.75\,10^5$	50	6.7×10^{-5}	2.4×10^{-4}	5774	704.0
5	$3.00\,10^6$	100	2.9×10^{-8}	1.3×10^{-7}	5418	3768.8
5	$1.01\,10^7$	150	1.2×10^{-11}	4.4×10^{-11}	5251	11489.8
5	$3.19\,10^7$	220	2.3×10^{-12}	3.1×10^{-12}	5410	36594.8

the truncated kernel method of [35] can provide explicit matrix entries) or a preconditioning strategy suitable for this class of problems. We are currently investigating both lines of research and will report on our progress at a later date. Another direction for further research is to relax the assumptions about the anisotropic material parameters, which here have been assumed to be matrices whose eigenvalues have positive real parts and nonnegative imaginary parts. In particular, our results do not apply in their present form to negative index materials.

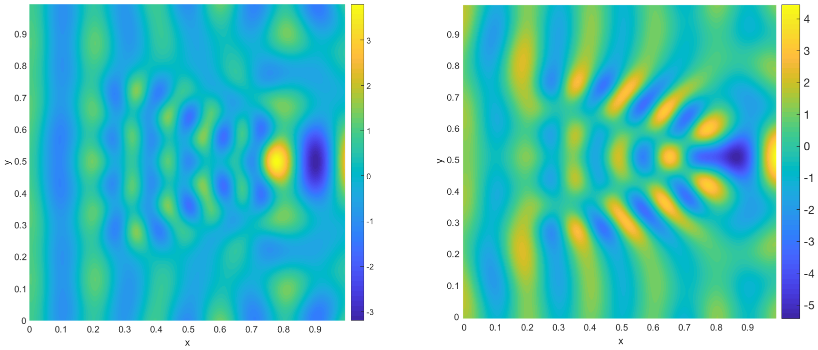

Fig. 3. *A slice of the z-component of the electric field at $z = 1/2$ (left) when solving the Maxwell scattering problem with $\omega = 10\pi$, $\mu = I$, and $\epsilon = \epsilon_{dense}$ defined in* (4.3) *using a* $150\times150\times150$ *grid. A slice of the real part of the acoustic field at $z = 1/2$ (right) when solving the Helmholtz scattering problem with $\omega = 10\pi$, and $\epsilon = \epsilon_{234}$ defined in* (4.2) *using a* $150 \times 150 \times 150$ *grid.*

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