A Completely Iterative Method for the Infinite Domain Electrostatic Problem with Nonlinear Dielectric Media

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Abstract

We present an iterative method for the solution of the exterior all-space electrostatic problem for nonlinear dielectric media. The electric potential is specified on interior boundaries and the electric field decays at infinity. Our approach uses a natural variational formulation based on the total energy of the nonlinear dielectric medium subject to boundary conditions. The problem is decomposed into an exterior calculation and an interior calculation with the boundary-specified electric potentials imposed as constraints between them. Together, these enable an iterative method that is based on the variational formulation. In contrast to direct solution of the electrostatic problems, we avoid the construction, storage and solution of dense and large linear systems. This provides important advantages for multiphysics problems that couple the linear electrostatic Poisson problem to nonlinear physics: the latter necessarily involves iterative approaches, and our approach replaces a large number of direct solves for the electrostatics with an iterative algorithm that can be coupled to the iterations of the nonlinear problem. We present examples applying the method to inhomogeneous, anisotropic nonlinear dielectrics. A key advantage of our variational formulation is that we require only the free-space, isotropic, homogeneous Greens function for all these settings.

Keywords: exterior electrostatics problem; nonlinear anisotropic inhomogeneous dielectrics; Dirichlet-to-Neumann map; multiphysics coupling

1 Introduction

Exterior electrostatic problems occur in a variety of engineering settings such as in MEMS, electronics, and NEMS. These settings often involve complex boundary conditions and geometries. For example, a common thin-film device geometry uses inter-digitated electrodes on the surface; these specify the voltage on electrodes while free-surface boundary conditions are used elsewhere. In general, the combination of free surfaces and electrodes with specified voltage allow the electric field to extend outside the device over all space, thus leading to an exterior electrostatic problem. In addition to this complexity, modern engineering materials can have strongly nonlinear dielectric responses in the regimes of interest. This

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setting of exterior electrostatic problems with complex boundary conditions in the presence of material nonlinearity motivates our work. It requires the solution of a linear electrostatics (Poisson) problem that is coupled to the nonlinear material response problem. The material response provides the charge that appears in the Poisson equation, while it in turn depends nonlinearly on the electric field that appears from solving the Poisson equation.

Though the electrostatic problem is formulated on all space, only the electric field in some region near the electrodes is typically of interest. This has led to a number of approaches that use ideas such as the Boundary Element Method (BEM) [14, 11] and the Dirichlet-to-Neumann map [2]. A common approach replaces the specified voltage on the electrodes with a consistent surface charge distribution that is calculated using the Greens function for the all-space Poisson problem [1, 15, 6, 9]. However, these are restricted to the setting where the charge distribution is *specified*, rather than evolving due to the nonlinear response of the dielectric medium. Recently, they have extended to the nonlinear setting [3], but with a direct approach, while the coupled nonlinear response of the dielectric necessarily uses an iterative approach. Hence, a direct solve[1] is required at every iterative update of the coupled nonlinear problem. The direct solve uses fully-populated matrices and Greens function integrations over the domain and it is prohibitively expensive for realistic nonlinear coupled problems.

A recent work [10] uses an iterative approach for the exterior electrostatics problem. While iterative, it deals with the case of specified charge distribution. In this work, we develop a completely iterative approach to the coupled problems of exterior electrostatics and nonlinear dielectrics. Our approach builds on [10] with some important differences. We begin by identifying a natural min-max variational formulation for the full problem and using this to provide an iteration towards stationary points. We split the electric fields into interior and exterior and apply the coupling conditions as constraints, in spirit similar to domain decomposition approaches [8]. Due to the completely iterative nature of our algorithm, we avoid the need to deal with the complexities of the inf-sup condition. We present examples that demonstrate the use of our algorithm to nonlinear, inhomogeneous and anisotropic dielectric media. An essential aspect of our variational formulation is that the electrostatic problem is *always* linear, homogeneous and isotropic, while the nonlinearity, inhomogeneity and anisotropy are confined to the nonlinear material response. This enables us to use the all-space homogeneous, isotropic Greens function kernel in all of these complex settings, rather than difficult and expensive numerical calculations of Greens functions for each case.

Our paper is organized as follows. The problem setting and the variational formulation are in Section 2, the decomposition into external and internal fields and derivation of the algorithm are in Section 3, a summary of the numerical implementation and a formal comparison with direct approaches are in Section 4, numerical examples are presented in Section 5, and we conclude in Section 6.

2 Problem Setting and the Variational Formulation

Consider a dielectric material occupying Ω with boundary $\partial\Omega$ and outward normal $\boldsymbol{n}$ as shown in Figure 1. A fixed surface potential ϕ^* is prescribed on part of the boundary S_1. The boundary $S_2 := \partial\Omega \backslash S_1$ is the free surface. The electric field $\nabla\phi$ decays at infinity. The region of interest may correspond to Ω or

[1] By direct solve, we mean that the system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ is solved for $\boldsymbol{x}$ exactly at every iteration, with $\boldsymbol{b}$ being updated at every iteration. While this is often not expensive, e.g., when LU decompositions are computed once and stored, in the exterior electrostatics case the Greens function integration makes this extremely expensive.

some larger region. For later use, we define $\overline{\Omega} := \mathbb{R}^3 \backslash \Omega$.

The total potential energy E of Ω is a functional of the polarization field $\boldsymbol{p}(\boldsymbol{x})$ induced the body and the electrostatic potential $\phi(\boldsymbol{x})$ in all space [13]:

$$E[\boldsymbol{p}, \phi] = \min_{\boldsymbol{p},\phi} \int_\Omega W(\boldsymbol{p})\, d\Omega + \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} |\nabla\phi|^2\, d\Omega \tag{2.1}$$

where W is the stored energy density of the material and is a function of polarization $\boldsymbol{p}$, and ϵ_0 is the permittivity of free space. The second term is the electrostatic field energy that is present over all space and is calculated by solving the electrostatic equation:

$$\epsilon_0 \nabla \cdot \nabla\phi = \nabla \cdot \boldsymbol{p} =: \rho_b \text{ over } \mathbb{R}^3 \tag{2.2}$$

subject to boundary conditions on ϕ, as well as $\epsilon[\![\nabla\phi]\!] \cdot \boldsymbol{n} = \boldsymbol{p} \cdot \boldsymbol{n} =: \sigma_b$ on the free surfaces S_2. The brackets $[\![\cdot]\!]$ denote the jump in a quantity across the boundary $\partial\Omega$. This is obtained by considering the integral statement of electrostatics when the electric field $\nabla\phi$ is discontinuous across the boundary (we note that that ϕ is continuous). The quantities σ_b and ρ_b denote the bound surface and volume charge densities respectively.

In the specific case $W \equiv 0$, we obtain the standard electrostatics problem with charge density specified. In the case $W = \frac{\epsilon_0}{2} \boldsymbol{p} \cdot \boldsymbol{\chi} \cdot \boldsymbol{p}$, we obtain the standard linear dielectric medium with dielectric permittivity $\boldsymbol{\epsilon} = \epsilon_0 (\boldsymbol{I} + \boldsymbol{\chi})$. Generically, W is a nonlinear function of $\boldsymbol{p}$. A recent approach uses the variational statement (2.1) to set up an iterative descent algorithm; however this requires the solution of the electrostatic constraint at every iteration [3]. Though the constraint is linear, it is nonlocal and expensive.

The alternate approach that we propose in this paper is to modify the variational statement to incorporate the constraint, following ideas from micromagnetism [7]. This variational statement is now a min-max statement but without the separate electrostatic constraint:

$$E[\boldsymbol{p}, \phi] = \min_{\boldsymbol{p}} \max_{\phi} \int_\Omega \left(W(\boldsymbol{p}) + \nabla\phi \cdot \boldsymbol{p}\right)\, d\Omega - \frac{\epsilon_0}{2} \int_{\mathbb{R}^3} |\nabla\phi|^2\, d\Omega \tag{2.3}$$

Computing the quantity $\delta E = E[\boldsymbol{p} + \epsilon\boldsymbol{q}, \phi + \epsilon\psi] - E[\boldsymbol{p}, \phi]$ and retaining only terms linear in ϵ, we obtain

$$\delta E = \int_\Omega \left(\frac{dW}{d\boldsymbol{p}} + \nabla\phi\right) \cdot \epsilon\boldsymbol{q}\, d\Omega + \int_{\mathbb{R}^3} \left(\epsilon_0 \nabla^2\phi - \nabla \cdot \boldsymbol{p}\right) \epsilon\psi\, d\Omega + \int_{S_2} \left(-\epsilon_0 [\![\nabla\phi \cdot \boldsymbol{n}]\!] + \boldsymbol{p} \cdot \boldsymbol{n}\right) \epsilon\psi\, dS \tag{2.4}$$

where the third integral is due to integrating-by-parts on $\nabla\psi \cdot \boldsymbol{p}$. Requiring E to be stationary with respect to ϕ and $\boldsymbol{p}$, we obtain the equilibrium equations:

$$\begin{aligned} \frac{dW}{d\boldsymbol{p}} + \nabla\phi &= 0 \text{ on } \Omega \\ \epsilon_0 \nabla^2\phi(\boldsymbol{x}) = \nabla \cdot \boldsymbol{p} &= \rho_b(\boldsymbol{x}) \text{ over } R^3 \\ \epsilon_0 [\![\nabla\phi(\boldsymbol{x})]\!] \cdot \boldsymbol{n} = \boldsymbol{p} \cdot \boldsymbol{n} &= \sigma_b(\boldsymbol{x}) \text{ on } S_2 \\ \phi(\boldsymbol{x}) &= \phi^*(\boldsymbol{x}) \text{ on } S_1 \end{aligned} \tag{2.5}$$

Equation $(2.5)_1$ is the constitutive relationship that provides the polarization response of the medium to electric field, and $(2.5)_{2,3,4}$ are the governing equation and boundary conditions of the electrostatics problem. All the anisotropy and inhomogeneity in the problem is now contained in the function W thus enabling the use of the well-known free-space Greens function for the electrostatics.

3 Solution Decomposition and the Iterative Algorithm

We begin by decomposing ϕ into $\phi_1 + \phi_2$ following [10], as shown in Figure 2. The field $\phi_1 = 0$ on $\partial\Omega$ and $\overline{\Omega}$, while ϕ_2 can be nonzero both on Ω and $\overline{\Omega}$. At this point, the decomposition is not unique. We also introduce a Lagrange Multiplier μ to enforce the Dirichlet boundary condition $\phi = \phi^*$ on S_1. The energy E is then:

$$\begin{aligned} E = &\int_\Omega W(\boldsymbol{p})\, d\Omega - \frac{\epsilon_0}{2}\int_\Omega |\nabla\phi_1|^2\, d\Omega - \frac{\epsilon_0}{2}\int_{\mathbb{R}^3} |\nabla\phi_2|^2\, d\Omega - \frac{\epsilon_0}{2}\int_\Omega 2\nabla\phi_1\cdot\nabla\phi_2\, d\Omega \\ &+ \int_\Omega \nabla(\phi_1+\phi_2)\cdot\boldsymbol{p}\, d\Omega - \int_{S_1}\mu(\phi_2-\phi^*)\, dS \end{aligned} \tag{3.1}$$

The variation of the energy E with respect to $\boldsymbol{p}$ is:

$$\frac{\delta E}{\delta \boldsymbol{p}} = \int_\Omega \left(\frac{dW}{d\boldsymbol{p}} + \nabla\phi\right)\, d\Omega \tag{3.2}$$

This provides a descent direction with respect to $\boldsymbol{p}$:

$$\dot{\boldsymbol{p}} \sim -\frac{dW}{d\boldsymbol{p}} - \nabla(\phi_1+\phi_2), \tag{3.3}$$

where $\dot{\boldsymbol{p}}$ is the increment in $\boldsymbol{p}$ and can be considered as the time-derivative in a gradient flow. We note that this is not a PDE but is defined point-wise and hence there are no boundary conditions associated to this.

Similarly, for ϕ_1 and ϕ_2,

$$\begin{aligned} \delta E = &\int_\Omega \left(\epsilon_0\nabla^2\phi_1 + \epsilon_0\nabla^2\phi_2 - \nabla\cdot\boldsymbol{p}\right)\, \delta(\phi_1+\phi_2)\, d\Omega + \int_{\overline{\Omega}} \epsilon_0\nabla^2\phi_2\, \delta\phi_2\, d\Omega \\ &- \int_{S_1}\mu\,\delta\phi_2\, dS - \int_{\partial\Omega}\left(\epsilon_0[\![\nabla\phi_2\cdot\boldsymbol{n}]\!] - \epsilon_0\nabla\phi_1\cdot\boldsymbol{n} + \boldsymbol{p}\cdot\boldsymbol{n}\right)\, \delta\phi_2\, dS \end{aligned} \tag{3.4}$$

This provides the ascent direction with respect to $\phi = \phi_1 + \phi_2$:

$$\begin{aligned} \dot{\overline{\phi_1+\phi_2}} &\sim \epsilon_0(\nabla^2\phi_1 + \nabla^2\phi_2) - \nabla\cdot\boldsymbol{p} \text{ on } \Omega \\ \dot{\phi_2} &\sim \epsilon_0\nabla^2\phi_2 \text{ on } \overline{\Omega} \end{aligned} \tag{3.5}$$

We recall that the decomposition $\phi = \phi_1 + \phi_2$ is not unique as yet. We exploit the linearity of the Laplacian operator and make the choice below for efficiency.

$$\begin{aligned} \dot{\phi_1} &= \epsilon_0\nabla^2\phi_1 - \nabla\cdot\boldsymbol{p} \text{ on } \Omega \\ \phi_1 &= 0 \text{ on } \partial\Omega \end{aligned} \tag{3.6}$$

Thus, the equation for ϕ_2 is

$$\begin{aligned} &\dot{\phi_2} \sim \epsilon_0\nabla^2\phi_2 \text{ on } \mathbb{R}^3 \\ &\epsilon_0[\![\nabla\phi_2\cdot\boldsymbol{n}]\!] = -\epsilon_0\nabla\phi_1\cdot\boldsymbol{n} + \boldsymbol{p}\cdot\boldsymbol{n} \text{ on } S_2 \\ &\epsilon_0[\![\nabla\phi_2\cdot\boldsymbol{n}]\!] = -\mu - \epsilon_0\nabla\phi_1\cdot\boldsymbol{n} + \boldsymbol{p}\cdot\boldsymbol{n} \text{ on } S_1 \end{aligned} \tag{3.7}$$

This reason for our specific choice is that it eliminates the Greens functions integrations over the interior. In particular, ϕ_1 is now a standard Dirichlet problem on a finite domain with forcing $\nabla \cdot \boldsymbol{p}$. While ϕ_2 still require Greens function integration, it is only over $\partial\Omega$. This is also illustrated in terms of linear operator formalism around (4.4). The choice of boundary condition $\phi_1 = 0$ on $\partial\Omega$ is for convenience; the choice $\phi_1 = V_0(\boldsymbol{x})$ is also possible, but would then require compensating dipoles on $\partial\Omega$ to ensure that $\phi_1 = 0$ on $\overline{\Omega}$.

To update $\boldsymbol{p}$, we need ϕ only inside Ω, and hence we express ϕ_2 on $\partial\Omega$ as

$$\bar{\phi} = \int_{S_1} (-\mu - \epsilon_0 \nabla\phi_1 \cdot \boldsymbol{n} + \boldsymbol{p} \cdot n)\, G(\boldsymbol{x}, \boldsymbol{x}')\, dS + \int_{S_2} (-\epsilon_0 \nabla\phi_1 \cdot \boldsymbol{n} + \boldsymbol{p} \cdot \boldsymbol{n})\, G(\boldsymbol{x}, \boldsymbol{x}')\, dS \tag{3.8}$$

using the all-space, isotropic, homogeneous Greens function $G(\boldsymbol{x}, \boldsymbol{x}')$. Then, we can update ϕ_2 using

$$\begin{aligned} \dot{\phi_2} &\sim \epsilon_0 \nabla^2 \phi_2 \text{ on } \Omega \\ \phi_2 &= \bar{\phi} \text{ on } \partial\Omega \end{aligned} \tag{3.9}$$

Finally, we obtain the equation for μ:

$$\frac{\delta E}{\delta \mu} = -\int_{S_1} (\phi_2 - \phi^*)\, dS_1 \Rightarrow \dot{\mu} \sim -\phi_2 + \phi^* \text{ on } S_1 \tag{3.10}$$

The Lagrange multiplier has the physical interpretation of the consistent charges that are required on the electrodes to satisfy the voltage boundary conditions.

4 Numerical Implementation

The iterative method begins with initial guesses for $\boldsymbol{p}$, ϕ_1, ϕ_2 and μ and computes their evolution using (3.3,3.5,3.9,3.10) until a stationary point is reached. We discretize using linear triangle elements for the evolution of $\phi_1, \phi_2, \boldsymbol{p}$ and standard boundary elements to discretize the boundaries. In this context, the iterative approach to the saddle-point variational formulation provides another advantage. The inf-sup restrictions are not applicable here and hence we are able to use the same discretization for all these fields and recycle the data structures and other calculations.

We formally compare our iterative algorithm with the direct approach. In the direct method, one solves for the consistent surface charge σ on the electrodes that satisfy the specified voltage boundary condition. Once σ is known, and given the bound charge surface and volume charges σ_b and ρ_b respectively, we can find ϕ using standard finite-domain methods for the Poisson equation with Dirichlet boundary conditions. Writing this in linear operator formalism, direct solution methods solve the equation:

$$\begin{Bmatrix} \phi_k \\ \phi_u \\ \phi_{int} + (\nabla^2)^{-1}[B_1\phi_k + B_2\phi_u] \end{Bmatrix} = \begin{bmatrix} \begin{bmatrix} \boldsymbol{G}_{11} & \boldsymbol{G}_{12} \\ \boldsymbol{G}_{21} & \boldsymbol{G}_{22} \end{bmatrix} & \bar{\boldsymbol{G}} \\ 0 & (\nabla^2)^{-1} \end{bmatrix} \times \begin{Bmatrix} \sigma_u \\ \sigma_k \\ \rho \end{Bmatrix} \tag{4.1}$$

where ϕ_k, σ_u are the (given) potential and (unknown) surface charge density on the electrodes S_1; ϕ_u, σ_k are the (unknown) potential and (given) surface charge density on the free surfaces S_2; and ϕ_{int}, ρ are the (unknown) potential and given volume charge density in Ω.

The operator $\bar{\boldsymbol{G}}$ is defined through

$$\bar{\boldsymbol{G}} \cdot \boldsymbol{\rho} = \int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}') \rho\left(\boldsymbol{x}'\right) d\boldsymbol{x}' \tag{4.2}$$

This is essentially a Greens function integration, and construction of and forward operations on this matrix are expensive even with fast multipole methods.

The operators B_1 and B_2 formally represent the linear relations between the boundary conditions and the ϕ_{int}. The operator $\boldsymbol{G}$ is defined as

$$\boldsymbol{G} \cdot \boldsymbol{\sigma} = \begin{bmatrix} \boldsymbol{G}_{11} & \boldsymbol{G}_{12} \\ \boldsymbol{G}_{21} & \boldsymbol{G}_{22} \end{bmatrix} \cdot \begin{Bmatrix} \sigma_u \\ \sigma_k \end{Bmatrix} = \int_{S} G(\boldsymbol{x}, \boldsymbol{x}') \sigma\left(\boldsymbol{x}'\right) d\boldsymbol{x}' \tag{4.3}$$

We decompose (4.1) into the following sum:

$$\begin{aligned} \begin{Bmatrix} 0 \\ 0 \\ \phi^1_{int} \end{Bmatrix} &= \begin{bmatrix} \begin{bmatrix} \boldsymbol{G}_{11} & \boldsymbol{G}_{12} \\ \boldsymbol{G}_{21} & \boldsymbol{G}_{22} \end{bmatrix} & \bar{\boldsymbol{G}} \\ 0 & (\nabla^2)^{-1} \end{bmatrix} \cdot \begin{Bmatrix} \sigma^*_u \\ \sigma^*_k \\ \rho \end{Bmatrix} \\ \begin{Bmatrix} \phi_k \\ \phi_u \\ \phi^2_{int} + (\nabla^2)^{-1}[A_1\phi_k + A_1\phi_u] \end{Bmatrix} &= \begin{bmatrix} \begin{bmatrix} \boldsymbol{G}_{11} & \boldsymbol{G}_{12} \\ \boldsymbol{G}_{21} & \boldsymbol{G}_{22} \end{bmatrix} & \bar{\boldsymbol{G}} \\ 0 & (\nabla^2)^{-1} \end{bmatrix} \cdot \begin{Bmatrix} \sigma_u - \sigma^*_u \\ \sigma_k - \sigma^*_k \\ 0 \end{Bmatrix} \end{aligned} \tag{4.4}$$

This decomposition enables us to avoid the construction of and forward multiplication with the fully populated matrix $\bar{\boldsymbol{G}}$. The last row of $(4.4)_1$ is a homogeneous Dirichlet problem that is efficiently solved for ϕ^1_{int} independent of the other two rows. In $(4.4)_2$, $\bar{\boldsymbol{G}}$ plays no role and hence we can efficiently solve for ϕ^2_{int}. The key issue is to find σ^*_u, σ^*_k efficiently.

Our method finds σ^*_u, σ^*_k through the following calculation. The first and second rows of $(4.4)_1$ imply that:

$$\int_{S_1} G(\boldsymbol{x}, \boldsymbol{x}') \sigma^*_u(\boldsymbol{x}') \, d\boldsymbol{x}' + \int_{S_2} G(\boldsymbol{x}, \boldsymbol{x}') \sigma^*_k(\boldsymbol{x}') \, d\boldsymbol{x}' = -\int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}') \rho(\boldsymbol{x}') \, d\boldsymbol{x}' \quad \forall \boldsymbol{x} \in \Omega \tag{4.5}$$

Using integration-by-parts on the right side:

$$\begin{aligned} -\int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}') \rho(\boldsymbol{x}') \, d\boldsymbol{x}' &= -\int_{\Omega} G(\boldsymbol{x}, \boldsymbol{x}') \nabla^2 \phi_1 \, d\boldsymbol{x}' \\ &= -\int_{\partial\Omega} [\![\nabla \phi_1 \cdot \boldsymbol{n}]\!] G(\boldsymbol{x}, \boldsymbol{x}') \, d\boldsymbol{x}' + \int_{\Omega} \nabla \phi_1 \nabla G(\boldsymbol{x}, \boldsymbol{x}') \, d\boldsymbol{x}' \end{aligned} \tag{4.6}$$

Integrating by parts on the second term on the right side above:

$$\int_{\Omega} \nabla \phi_1 \nabla G(\boldsymbol{x}, \boldsymbol{x}') \, d\boldsymbol{x}' = -\int_{\Omega} \nabla^2 G(\boldsymbol{x}, \boldsymbol{x}') \phi_1 \, d\boldsymbol{x}' + \int_{S} \nabla G(\boldsymbol{x}, \boldsymbol{x}') \cdot \boldsymbol{n} \phi_1 \, d\boldsymbol{x}' \tag{4.7}$$

Both terms are 0 because $\phi_1 = 0 \forall \boldsymbol{x} \in \partial\Omega$.

Since $\phi_1 = 0$ outside Ω, we have $[\![\nabla \phi_1 \cdot \boldsymbol{n}]\!] = \nabla \phi_1 \cdot \boldsymbol{n}$ on $\partial\Omega$. Further, since this holds for all $\boldsymbol{x} \in \partial\Omega$, we obtain:

$$\begin{aligned} \sigma^*_u &= -\nabla \phi_1 \cdot \boldsymbol{n} \quad \text{on } S_1 \\ \sigma^*_k &= -\nabla \phi_1 \cdot \boldsymbol{n} \quad \text{on } S_2 \end{aligned} \tag{4.8}$$

5 Numerical examples

We discuss the solution of four examples that illustrate the application of the method to anisotropic, inhomogeneous problems. To automatically satisfy the principles of frame indifference [5], we assume that the energy density is of the form $W(\boldsymbol{p}) = \hat{W}(\boldsymbol{p}\cdot\boldsymbol{\chi}_1\cdot\boldsymbol{p}, \boldsymbol{p}\cdot\boldsymbol{\chi}_2\cdot\boldsymbol{p}, \ldots)$. The symmetric, positive-definite, second-order tensors $\boldsymbol{\chi}_i$ characterize the anisotropy of the medium; an isotropic medium would have $\boldsymbol{\chi}_i$ equal to the identity. Further, an isotropic, linear dielectric has $W(\boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{p}$ and a linear anisotropic dielectric has $W(\boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{\chi}\cdot\boldsymbol{p}$. Inhomogeneous media are represented through explicit position dependence of the energy density function.

The first example applies the method to a linear dielectric with both Dirichlet and Neumann boundary conditions in a rectangular domain. Figure 3(a) depicts the boundary conditions with fixed potential on the top and bottom of the domain, and a point charge on the right side. The sides are free surfaces and the electric field is not confined there. Figure 3(b),3(c) and 3(d) show the results of potential, electric field and polarization respectively.

The second example examines a dielectric with a nonlinear polarization response to electric field, with boundary conditions as in Figure 4. The top surface is roughly sinusoidal. We choose $W = \alpha|\boldsymbol{p}|^4$. Numerical solutions of potential (both inside and outside the domain), electric field and polarization are shown in Figure 4(b),4(c) and 4(d). Convergence results for different mesh density are shown in Table 1; we find second order convergence in both L_1 and L_2 norm.

The third example demonstrates the applicability to a linear anisotropic dielectric. The computational domain and boundary conditions are shown in Figure 5(a). We choose the energy density $W = \boldsymbol{p}\cdot\begin{bmatrix}\alpha_1 & 0\\ 0 & \alpha_2\end{bmatrix}\cdot\boldsymbol{p}$. Numerical results are provided in Figure 5(b),5(c) and 5(d).

The last example examines a nonlinear and inhomogeneous dielectric, with boundary conditions as in Figure 6. We use the energy density $W = \alpha|\boldsymbol{p}|^4(0.01 + \beta x_2)$ where x_2 is the vertical coordinate. Numerical results are provided in Figure 6(b),6(c) and 6(d).

We note that in all of these examples, we require only the all-space, homogeneous, isotropic Green's function despite the complexities of the dielectric media. This enables a simple strategy to calculate fields in regions outside by redefining the extent of the body to encompass the regions of interest and using $W = \frac{\epsilon_0}{2}|\boldsymbol{p}|^2$ to represent the empty space that is nominally part of the body. The Lagrange multiplier approach that we have used to enforce electrode voltages are just as applicable if the electrodes are in the interior of the computational domain. Also, while these examples were all in 2D, the extension to 3D is straightforward with the appropriate Greens function.

6 Conclusion

We have presented an iterative method to find the electrostatic field in nonlinear, anisotropic, inhomogeneous dielectric media with a mix of boundary conditions that lead to an exterior problem. The iterative nature enables straightforward strategies to couple the method to nonlinear physics, such as large deformation electromechanical systems [4] and semiconductor dopant behavior [16]. These other phenomena are nonlinear and require iterative methods; rather than direct solves at every iteration [12] that can be

expensive, the iterations required for the electrostatics can be coupled to the iterations required for the other phenomena.

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Figures

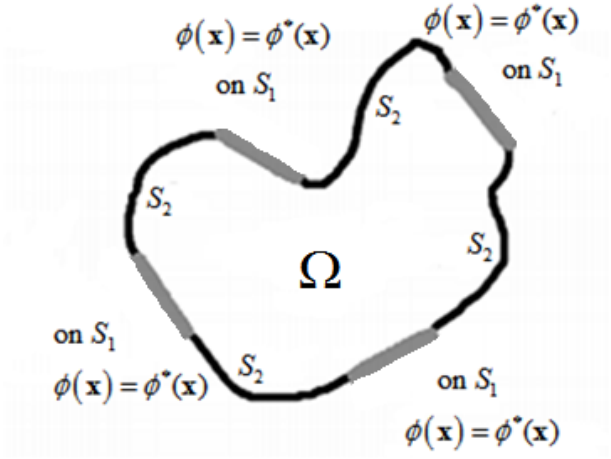


Figure 1: Formulation of the problem.

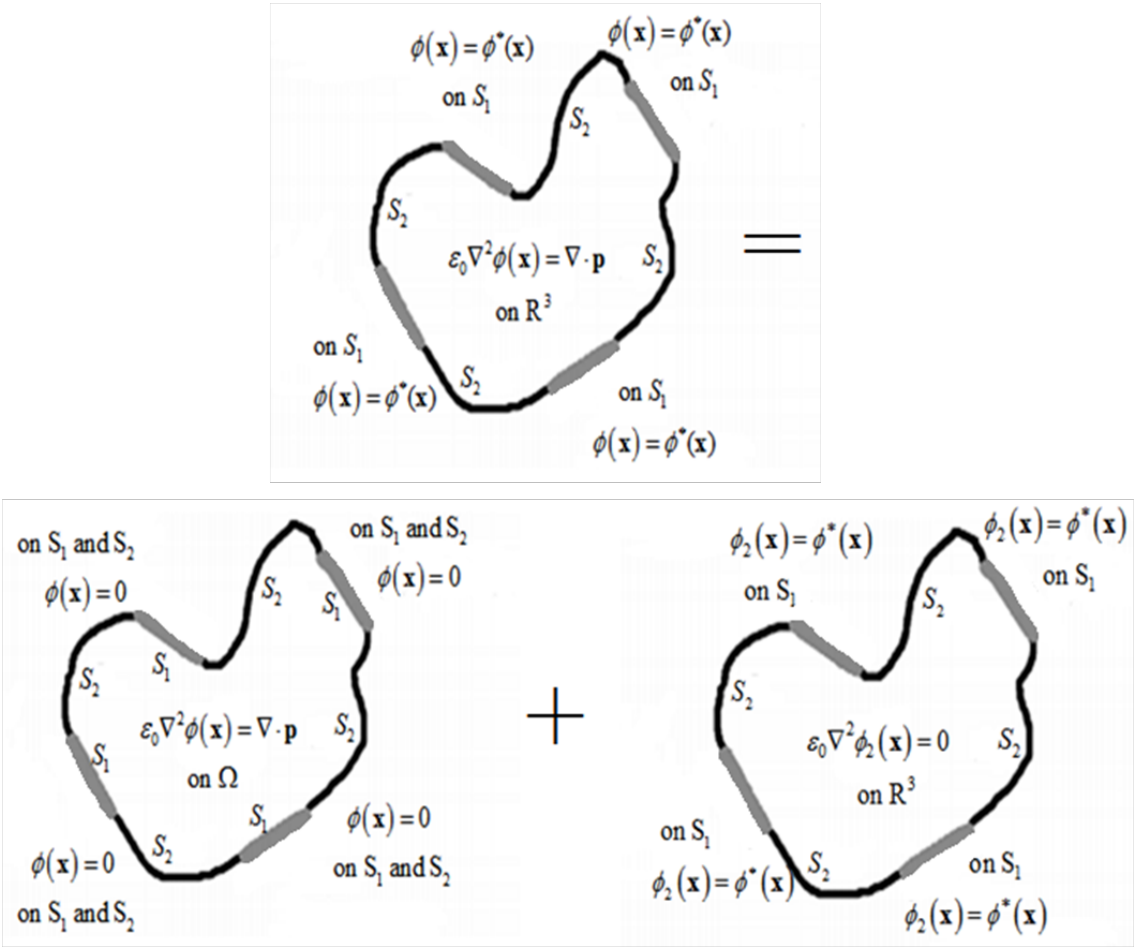
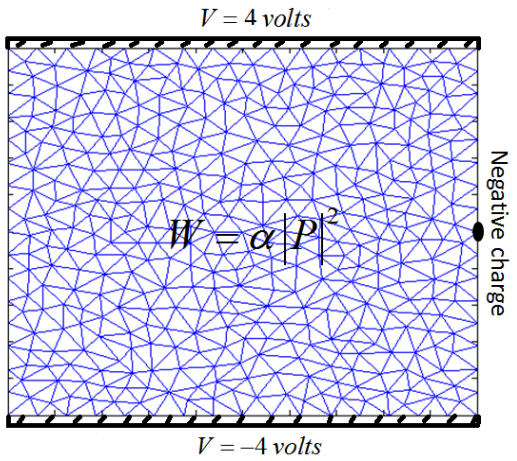
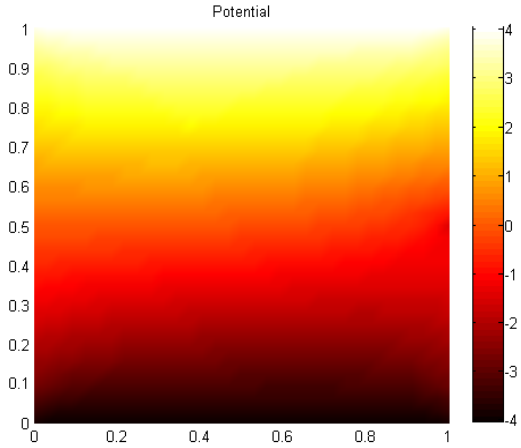


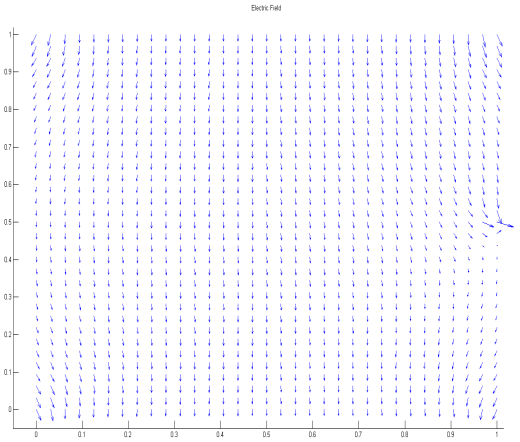
Figure 2: Decomposition into an interior problem and an exterior problem. The boundary condition for ϕ_2 on S_2 is $\epsilon_0[\![\nabla\phi_2\cdot\boldsymbol{n}]\!] = -\epsilon_0\nabla\phi_1\cdot\boldsymbol{n} + \boldsymbol{p}\cdot\boldsymbol{n}$.



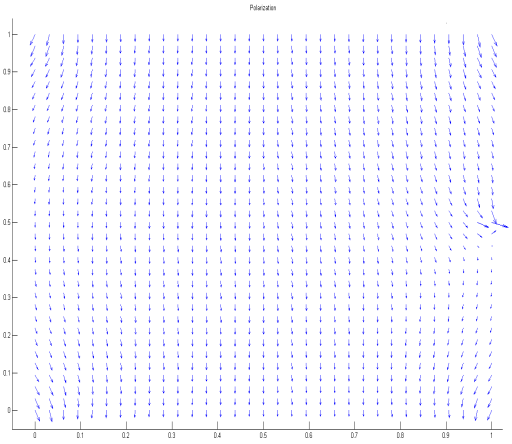
(a) Boundary conditions



(b) Potential



(c) Electric Field

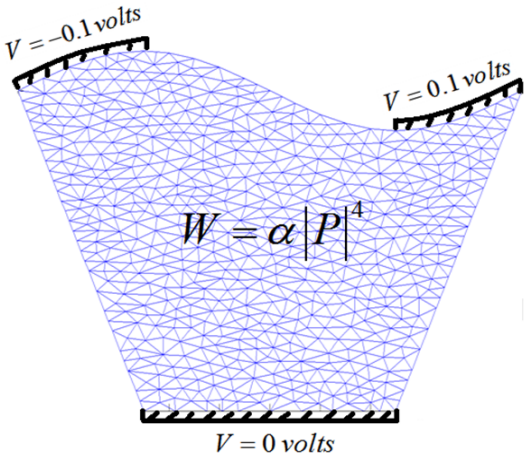


(d) Polarization

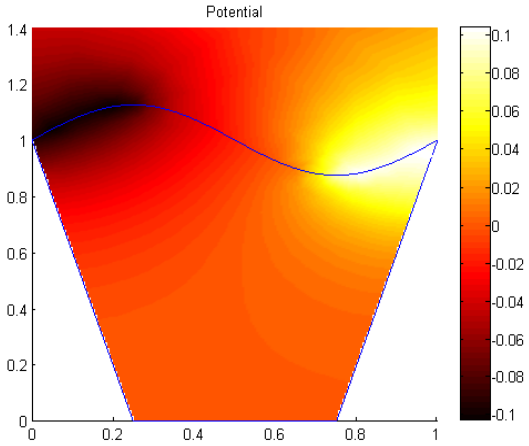
Figure 3: Example 1: Both Dirichlet and Neumann boundary conditions in a rectangular domain.

Table 1: Convergence study for nonlinear constitutive relations

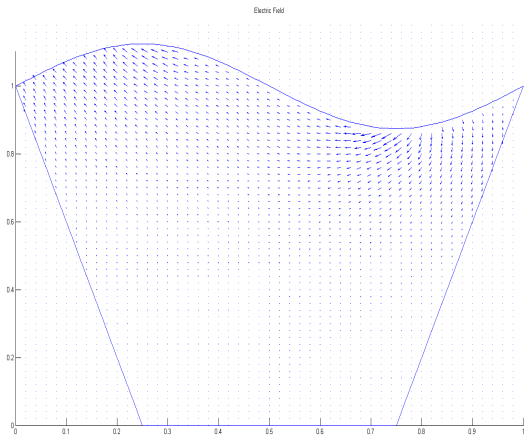
$\frac{1}{a}$	L_1	L_2
500	$1.061 * 10^1$	0.161
1000	$0.504 * 10^1$	0.084
2000	$0.233 * 10^1$	0.043



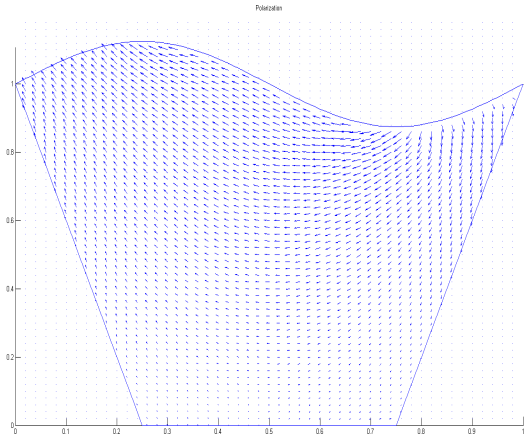
(a) Boundary conditions



(b) Potential

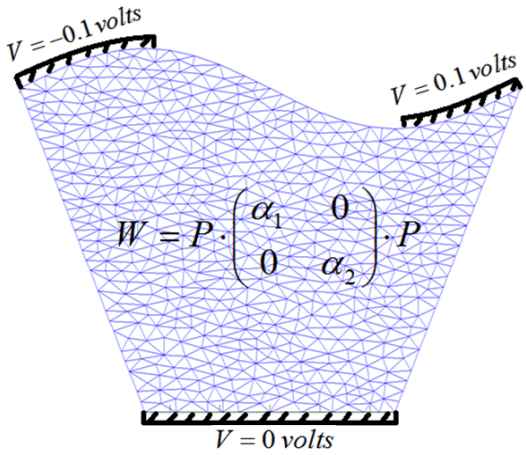


(c) Electric Field

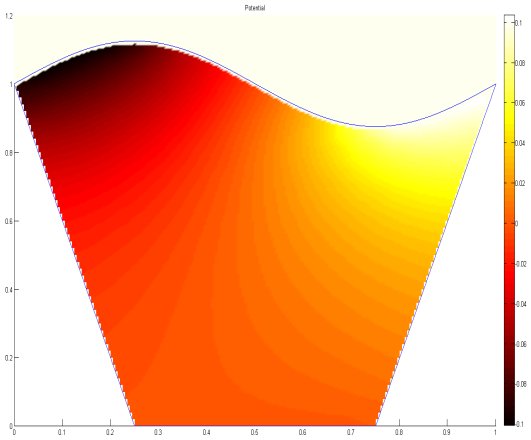


(d) Polarization

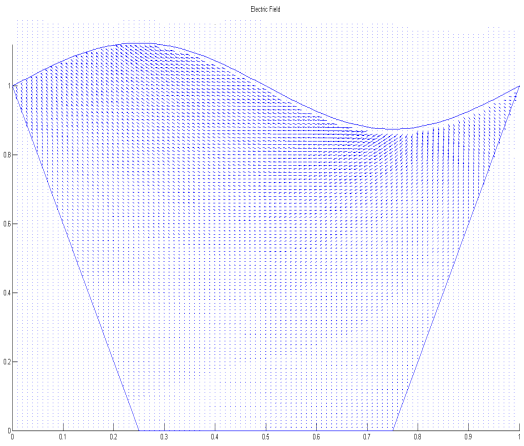
Figure 4: Example 2: A nonlinear dielectric with both Dirichlet and Neumann boundary conditions.



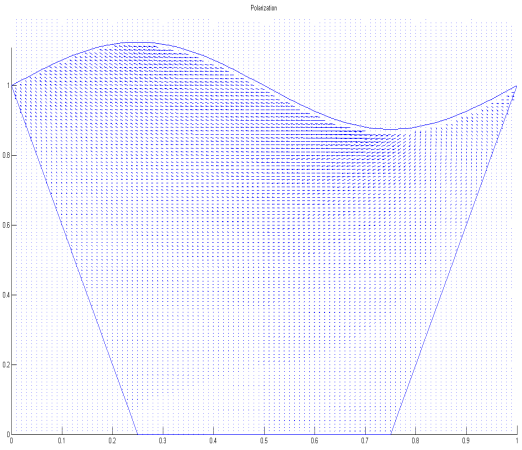
(a) Boundary conditions



(b) Potential

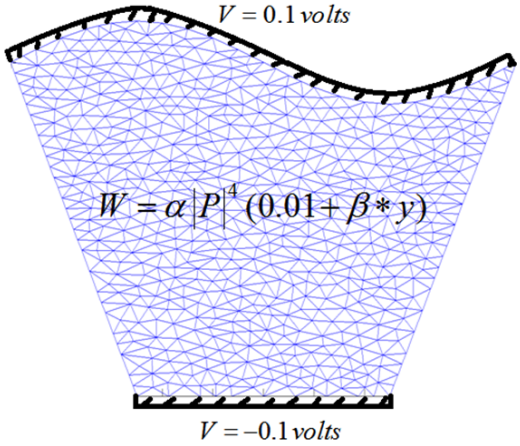


(c) Electric Field

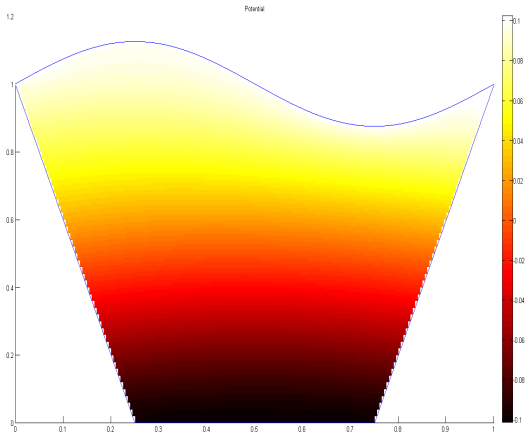


(d) Polarization

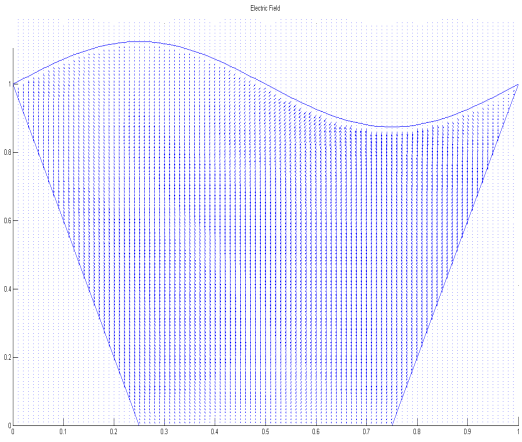
Figure 5: Example 3: A linear anisotropic dielectric with both Dirichlet and Neumann boundary conditions.



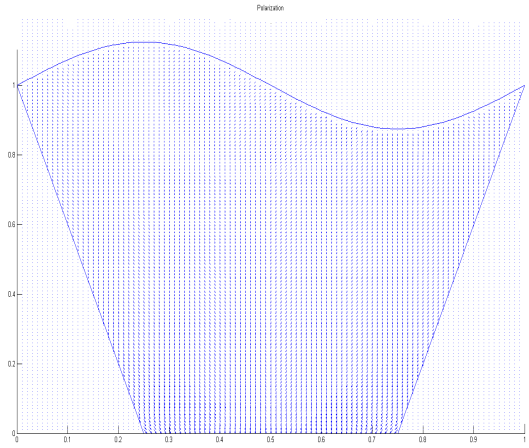
(a) Boundary conditions



(b) Potential



(c) Electric Field



(d) Polarization

Figure 6: Example 4: A nonlinear inhomogeneous dielectric with both Dirichlet and Neumann boundary conditions.