Inverse Design of Electromagnetic Devices using Topological Derivative Method

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ABSTRACT

An inverse design in electromagnetic method based on the topological derivative approach is presented. Topological derivative method is used to measure the sensitivity of a given functional with respect to an infinitesimal perturbation in a domain. The topological derivative concept has been successfully applied in many relevant fields such as geophysics, multi-scale material design and inverse problems. In this work, the reflection coefficient is considered as an objective function to design the electromagnetic devices. Finally, numerical experiments are presented to illustrate the performance of the optimisation approach.

Keywords: Electromagnetic scattering, Inverse problems, Topology Optimisation, Topological Derivatives

1. INTRODUCTION

Neutrinos are subatomic particles and one of the most abundant particles in the universe. However, they are difficult to detect, as they have weak interaction with matter. Detecting neutrinos and determining their absolute mass is an important goal in the particle physics field. To achieve this goal, it is necessary to develop sensor techniques capable of detecting low-power electronic signals. However, the development of effective and efficient design sensors is an engineering challenge, the complex dynamics of electromagnetic waves leads to non-intuitive designs. To overcome these challenges, topology optimisation methods are an essential part of this process. Thus, several topological optimisation methods in electromagnetic devices have been developed in recent years,[1,2] this approaches including bio-inspired methods,[3] level-set methods,[4,5] and adjoint-based methods.[6,7]

In this work, we present the topological derivative method applied to an electromagnetic scattering problem based on the work Ref. 8. Proposed by Sokołowski & Żochowski,[9] the main idea of the topological derivative method is to compute the variation of a functional that is associated with the topology of a given domain. In other words, because the functional is associated with the topology of a domain, the topological derivative identifies whether it is necessary to include or remove material at a given location. In particular, for this work, the reflection coefficient S_{lm} is chosen as an objective function to design the electromagnetic device. This functional is related to the topology of the domain, therefore, in a given region, the algorithm will measure its variation by changing a material Si for another SiO_2.

This paper is organized as follows: the electromagnetic scattering problem is defined in Section 2. The topological derivative method is introduced in Section 3. In addition, Section 4 presents a three spatial dimensions application example using reflexive coefficient as objective function. Finally, some basic mathematical definitions are described in Appendix A.

2. ELECTROMAGNETIC MODEL

Let us consider an open and bounded domain $\mathcal{D} \subset \mathbb{R}^3$. A near-field domain is denoted as $\mathcal{B}_R \subset \mathcal{D}$, with boundary $\Gamma = \partial\mathcal{B}_R$. The optimization region is given by $\Omega \subset \mathcal{B}_R$, such that $\Omega = \Omega_a \cup \Omega_b$ and $\Omega_a \cap \Omega_b = \emptyset$, with Ω_a and Ω_b representing regions with refractive index n_1 and n_2 respectively. As previously described, a generic domain is represented in Fig. 1.

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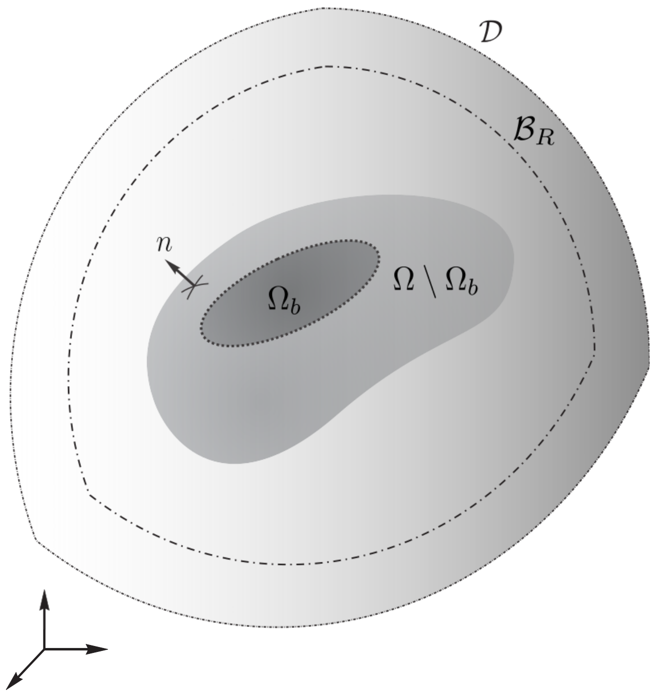

Figure 1. Generic representation of domain. The electromagnetic problem is defined $\mathcal{D}$. In addition, the near-field domain is defined as $\mathcal{B}_R \subset \mathcal{D}$. Finally, the optimization domain Ω is is split into two disjoints subdomains $\Omega_a = \Omega \setminus \Omega_b$ and Ω_b, which are represented by light and dark regions, respectively.

The electromagnetic wave scattering problem can be written mathematically as follows:

$$\left\{ \begin{array}{rcll} \nabla \times (\nabla \times E) - k_0^2 n_i^2 E &=& F, & \text{in } \mathcal{D}, \\ n \times E &=& 0, & \text{on } \Gamma_0, \\ n \times \nabla \times E &=& G_{\text{in}}, & \text{on } \Gamma_{\text{in}}, \\ n \times \nabla \times E &=& G_{\text{out}}, & \text{on } \Gamma_{\text{out}}, \end{array} \right. \tag{1}$$

where k_0 is the wavenumber in vacuum, n_i the refractive index, F is a source domain, n is the outward unit normal vector, G_{in} is the source of the input port and G_{out} is the source of the output port of the device $\mathcal{D}$.

The problem (1) can be compactly rewritten in a weak formulation: find $E \in \mathcal{V}$, such that

$$\int_{\mathcal{D}} \left(\nabla \times E \cdot \nabla \times W - k_0^2 n_i^2 E \cdot W \right) \mathrm{d}x = S(W), \quad \forall\, W \in \mathcal{V}, \tag{2}$$

where $S(W) \in \mathcal{V}'$ represents any boundary and domain source terms, with $\mathcal{V}'$ denoting the dual space of $\mathcal{V}$, the necessary definitions of space and norm among others are described in Appendix A.

3. THE TOPOLOGICAL DERIVATIVE METHOD

The topological derivative measures the sensitivity of a given shape functional with respect to an infinitesimal singular domain perturbation, such as the insertion of holes, inclusions, source-terms or even cracks. The topological derivative was rigorously introduced in Ref. 9. Since then, this concept has become a subject of intensive research. In fact, the topological derivative concept has proven to be useful, with a wide range of applications, such as image processing,[10] fracture[11] and damage[12] mechanics, seismic application[13] and treatment of cancer by hyperthermia.[14] For a deeper understanding, a detailed description of the method can be found in the books.[15,16]

Let us consider a characteristic function $\chi = \mathbb{1}_\Omega$ associated to the domain Ω. Suppose that Ω is subject to a singular perturbation confined in a small ball $B_\varepsilon(\widehat{x})$ of size ε and center at $\widehat{x} \in \Omega$, as shown in Fig. 2. We denote by $\chi_\varepsilon(\widehat{x})$

the characteristic function associated to the topologically perturbed domain. In the case of a perforation, for instance, $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{\overline{B_\varepsilon(\widehat{x})}}$, and the perforated domain is obtained as $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$. Then, we assume that a given shape functional $\psi(\chi_\varepsilon(\widehat{x}))$, associated to the topologically perturbed domain, admits the following topological asymptotic expansion

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + \rho(\varepsilon) D_T\psi(\widehat{x}) + \mathcal{R}(\rho(\varepsilon)), \tag{3}$$

where $\psi(\chi)$ is the shape functional associated to the original (unperturbed) domain, $\rho(\varepsilon)$ is a positive function such that $\rho(\varepsilon) \to 0$, when $\varepsilon \to 0$, and $\mathcal{R}(\rho(\varepsilon)) = o(\rho(\varepsilon))$ is the remainder. The function $\widehat{x} \mapsto D_T\psi(\widehat{x})$ is called the topological derivative of ψ at $\widehat{x}$. Therefore, this derivative can be seen as a first order correction of $\psi(\chi)$ to approximate $\psi(\chi_\varepsilon(\widehat{x}))$.

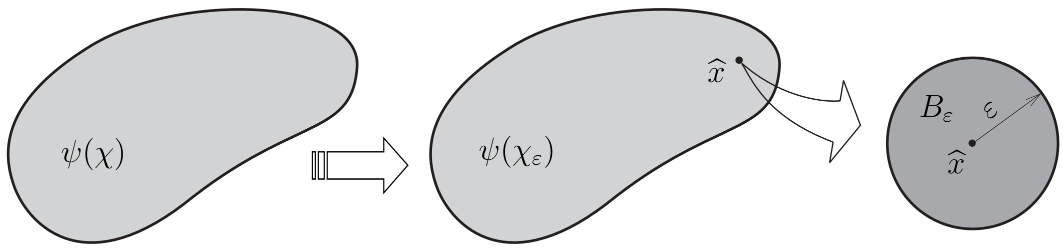

Figure 2. The topological derivative concept.

Since our goal is to maximize or minimize a shape functional given, in general form, by

$$\psi(E) = \langle \varphi(E), \varphi^*(E) \rangle, \tag{4}$$

where $\langle \cdot, \cdot \rangle$ is the standard internal product and $*$ is used to denote the complex conjugate.

To define the objective function in terms of scattering parameters $S_{\ell m}$, the input and output ports of the device must be defined over Γ. With the normalized input mode m excited, the coefficient can be calculated by projecting the electromagnetic fields onto the normalized output port mode (e_ℓ, h_ℓ):[17–19]

$$S_{\ell m} := \varphi_\ell(E_m) = \int_\Gamma (E_m \times h_\ell + e_\ell \times H_m) \cdot \hat{n} \, \mathrm{d}s = \int_\Gamma (E_m \times h_\ell + j_\ell \times \nabla \times E_m) \cdot \hat{n} \, \mathrm{d}s, \tag{5}$$

where E_m is used to denote the solution of the FEM formulation (2) with normalized mode m as a source, $\hat{n}$ is the unit normal vector field to Γ and

$$j_\ell = \frac{i}{k_0 \eta_0 \mu_r} e_\ell. \tag{6}$$

In addition $\varphi_\ell : \mathcal{V} \mapsto \mathbb{C}$ is a complex-valued scalar function, then $\langle \varphi_\ell^*(E_m), \varphi_\ell(E_m) \rangle = \varphi_\ell^*(E_m)\varphi_\ell(E_m)$. In this case, the adjoint problem (10) reads: find $V \in \mathcal{V}$, such that

$$\int_\mathcal{D} \left(\nabla \times V \cdot \nabla \times W - k_0^2 n^2 V \cdot W \right) \mathrm{d}x = \varphi_\ell^*(E_m) \int_\Gamma \left(h_\ell \times \hat{n} \cdot W + \hat{n} \times j_\ell \cdot \nabla \times W \right) \mathrm{d}s \quad \forall\, W \in \mathcal{V}. \tag{7}$$

In particular, in this work, the topological derivative represents the sensitivity of the shape functional $\psi(E)$ with respect to the nucleation of a small inclusion in Ω with different material properties. For this work the associated topological derivative is given by the following result:

PROPOSITION 3.1. *Let $\psi(E)$ be the shape functional (4), with E used to denote the solution to the variational problem (2). Then, its topological derivative can be written as*

$$D_T\psi(x) = 2\Re\{k_0^2(n_2^2 - n_1^2) s(x) E(x) \cdot V(x)\}, \tag{8}$$

for almost all $x \in \Omega$. The signal function $s(x)$ is given by

$$s(x) = \begin{cases} +1, & x \in \Omega_a \\ -1, & x \in \Omega_b \end{cases}. \tag{9}$$

and the adjoint state V is solution to the following auxiliary variational problem: find $V \in \mathcal{V}$, such that

$$\int_{\mathcal{D}} \left(\nabla \times V \cdot \nabla \times W - k_0^2 n_i^2 V \cdot W\right) \mathrm{d}x = \langle \varphi^*(E), \varphi(W) \rangle \quad \forall\, W \in \mathcal{V}. \tag{10}$$

Proof. The proof is presented in Ref. 8. □

4. NUMERICAL RESULTS

The optimization over several wavelengths can also be used to tailor the spectral response of the device beyond a flat curve. Specific filters can be designed using this feature. As an example, we design a compact diplexer that splits signals from the O and C bands using $\lambda = 1.55\,\mu\mathrm{m}$. In this case the objective function is

$$\Psi(\Omega) = \left(1 - |S_{21}(1.55\,\mu\mathrm{m})|^2\right)^2. \tag{11}$$

The optimization domain is a 3-d volume with area $2.0\,\mu\mathrm{m} \times 2.0\,\mu\mathrm{m}$ and thickness of $110\,\mathrm{nm}$. The Si waveguides connected to the device, shown in Fig. 4(b), have widths of $200\,\mathrm{nm}$ and the same thickness as the optimization volume. All surroundings are filled with SiO_2.

APPENDIX A. BASIC DEFINITIONS

Some definitions are necessary. , the space $\mathcal{V}$ is defined as

$$\mathcal{V} := \{W \in H_{\mathrm{curl}}(\mathcal{D}; \mathbb{C}^d) : \hat{n} \times W = 0 \text{ on } \Gamma\}, \tag{12}$$

where $H_{\mathrm{curl}}(\mathcal{D}; \mathbb{C}^d)$ is used to denote the standard complex-valued Hilbert space[20] of vector functions $W : \mathcal{D} \mapsto \mathbb{C}^d$, such that $W \in L^2(\mathcal{D}; \mathbb{C}^d)$ and $\nabla \times W \in L^2(\mathcal{D}; \mathbb{C}^d)$. The associated norms in $L^{2p}(\mathcal{D}; \mathbb{C}^d)$ and $H_{\mathrm{curl}}(\mathcal{D}; \mathbb{C}^d)$ are respectively defined as

$$\|W\|_{L^{2p}(\mathcal{D};\mathbb{C}^d)} := \left(\int_{\mathcal{D}} |W|^{2p} \,\mathrm{d}x\right)^{\frac{1}{2p}}, \quad \|W\|_{H_{\mathrm{curl}}(\mathcal{D};\mathbb{C}^d)} := \left(\int_{\mathcal{D}} (|W|^2 + |\nabla \times W|^2) \,\mathrm{d}x\right)^{\frac{1}{2}}, \tag{13}$$

where $|W|^{2p} := (W \cdot \overline{W})^p$ for $1 \leq p < \infty$, with $\overline{W}$ used to denote the complex conjugate of W. Note that the L^2-norm is obtained by setting $p = 1$ in the above equation (left). Outside $\mathcal{B}_R$, the formulation can be extended to include anisotropic and magnetic materials, as required when open domains are simulated with the help of perfectly matched layer (PML). The associated magnetic field is given by

$$H = \frac{i}{k_0 \eta_0 \mu_r} \nabla \times E \tag{14}$$

with η_0 the vacuum wave impedance, and μ_r the relative magnetic permeability (assumed constant and equal for all materials in the near-field domain).

The complex-valued, scalar or vector function $\varphi(E)$ is assumed to be linear with respect to its argument, namely

$$\varphi(\alpha U + V) = \alpha\, \varphi(U) + \varphi(V) \quad \forall\, U, V \in \mathcal{V},\ \alpha \in \mathbb{C}, \tag{15}$$

and it is written in terms of integrals concentrated on Γ. In this scenario, we aim to find the best material distribution within Ω, which means to find the optimal topology for the domains Ω_a and Ω_b.

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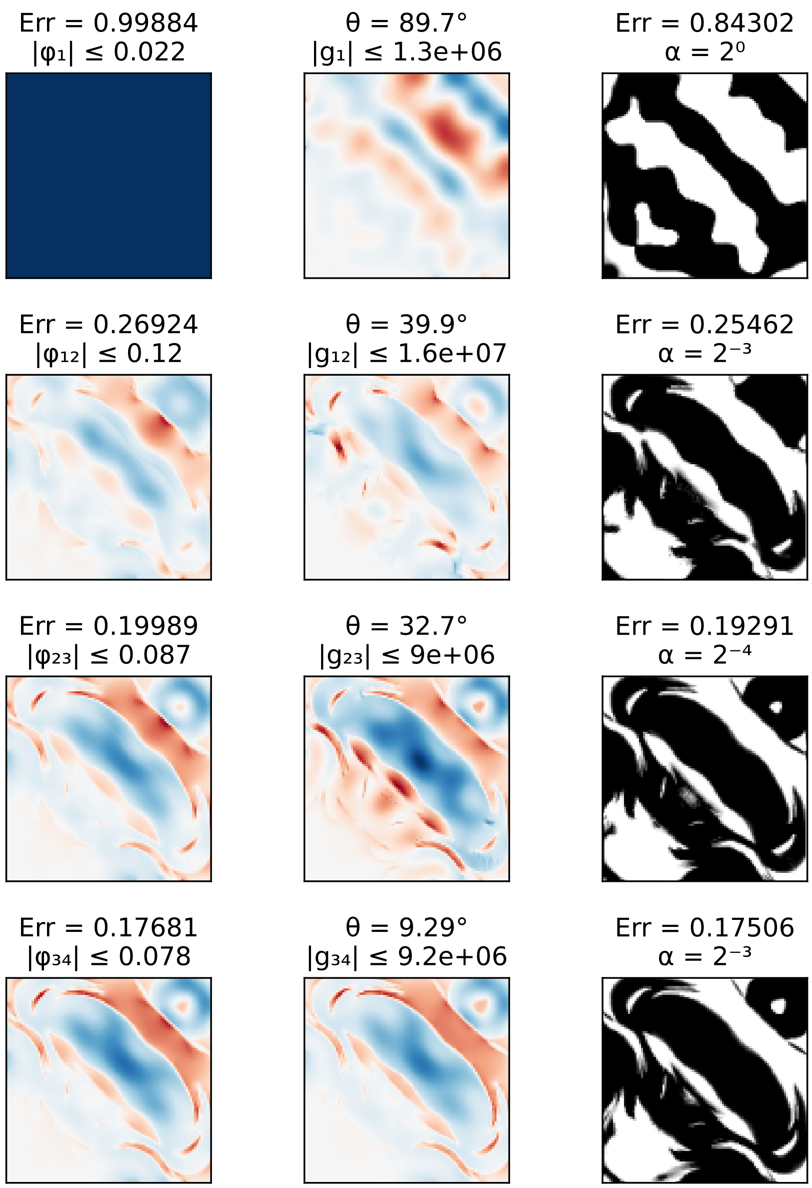
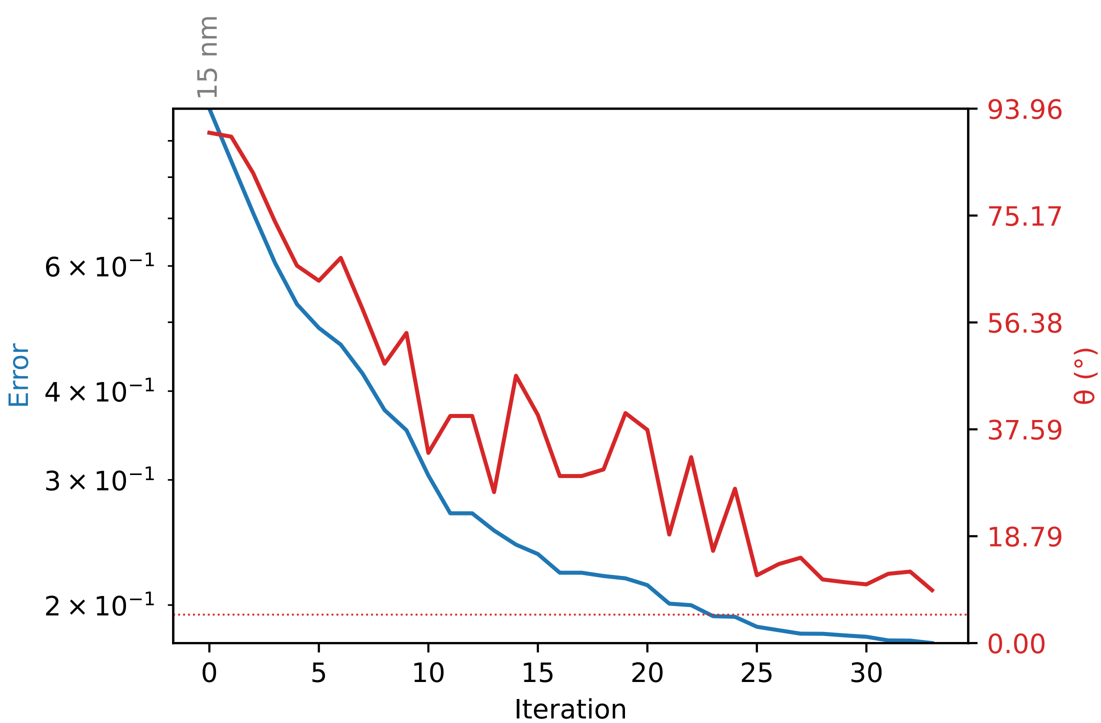

Err = 0.99884
$|\varphi_1| \le 0.022$
$\theta = 89.7°$
$|g_1| \le 1.3e+06$
Err = 0.84302
$\alpha = 2^0$
Err = 0.26924
$|\varphi_{12}| \le 0.12$
$\theta = 39.9°$
$|g_{12}| \le 1.6e+07$
Err = 0.25462
$\alpha = 2^{-3}$
Err = 0.19989
$|\varphi_{23}| \le 0.087$
$\theta = 32.7°$
$|g_{23}| \le 9e+06$
Err = 0.19291
$\alpha = 2^{-4}$
Err = 0.17681
$|\varphi_{34}| \le 0.078$
$\theta = 9.29°$
$|g_{34}| \le 9.2e+06$
Err = 0.17506
$\alpha = 2^{-3}$



15 nm
Error
6 × 10⁻¹
4 × 10⁻¹
3 × 10⁻¹
2 × 10⁻¹
0
5
10
15
20
25
30
Iteration
93.96
75.17
56.38
37.59
18.79
0.00
θ (°)

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