

SHAPE SENSITIVITY ANALYSIS OF ELECTRICALLY LARGE METALLIC ELECTROMAGNETIC SCATTERERS

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Abstract. *The electric field integral equation (EFIE) is an efficient boundary element method to simulate scattering of time-harmonic EM fields from metallic bodies. However, the pure EFIE can not be used to simulate electromagnetically large objects. Instead the multilevel fast multipole algorithm (MLFMA) must be used. In this paper an efficient method for computing the action of shape-differentiated electric field integral equation system matrix to a vector is derived exploiting MLFMA. The proposed method is used in conjunction with the adjoint-variable method to compute the gradient of an arbitrary objective function depending on the parameterized shape of a metallic scatterer.*

1 INTRODUCTION

Geometric (shape) optimization of high-performance antennas, such as those in hand-held mobile devices, is an important part of their design process [1]. Such optimization requires multiple simulations of the device for various geometric configurations, and therefore the joint effect of efficiencies of the simulation and optimization algorithms is quadratic on the time spent optimizing the device. Hence it is important that the underlying simulation algorithm is efficient and that the optimization process converges with as few iterations as possible.

Optimization methods can be generally classified into two categories based on whether they use gradient information or not. The main advantages of gradient-based optimization methods over non-gradient ones are that they typically converge with fewer evaluations of the cost function, and that the obtained design can be guaranteed to be a local optimum.

Applying difference formulas to the objective function is the most generic method to approximate the gradient. The shortcomings of this approach are that one must compute $M+1$ full system solutions, where M is the number of design variables, and the accuracy of the finite difference is sensitive to the step length.

The adjoint variable method (AVM) eases the computational burden of naive appliance of finite differences to the objective function by, roughly speaking, transferring the differentiation to the system matrix level. The system matrix can be differentiated using numerous methods such as the automatic differentiation (AD) [2, 3] or analytically by hand [4]. In the AVM, at most two large linear systems need to be solved: the state and the adjoint equations. Furthermore, being a purely algebraic method, the AVM applies to arbitrary objective functions.

The electric field integral equation is a widely used and efficient boundary element method to simulate scattering of time-harmonic electromagnetic fields from highly conducting metallic bodies or surfaces. Moreover, it is the de-facto method to compute electric characteristics of such antennas. However, being a boundary element method, its discretization results in a fully populated matrix which is a significant drawback if the model to be simulated is large. This obstacle can be overcome by utilizing the so called fast multipole methods.

In this work we present how the shape derivative of electrically large metallic structures can be computed efficiently with the multilevel fast multipole algorithm (MLFMA) using the adjoint variable method. At first sight the differentiation the system matrix seems impossible as it is not assembled and stored in the traditional way. However, we demonstrate that it is not a problem and discuss the implementational details on how a regular solver code needs to be changed to have it compute the shape derivatives.

2 STATE PROBLEM

Let us consider a 3D antenna structure in a free space and let us assume that the antenna structure can be modelled with open, possibly non-connected, metallic surface. We use the time-factor $e^{-i\omega t}$.

By denoting the surface of the antenna with Γ , and the primary exciting field \mathbf{E}^p , the electric field integral equation (EFIE) for the problem reads

$$\left[-i\omega\mu(\mathcal{S}\mathbf{J})(\mathbf{r}) + \frac{1}{i\omega\epsilon}\nabla(\mathcal{S}\nabla_{\Gamma}\cdot\mathbf{J})(\mathbf{r}) \right]_{\tan} = \left[\mathbf{E}^p(\mathbf{r}) \right]_{\tan}, \quad (1)$$

where $\mathbf{J} = \mathbf{n} \times \mathbf{H}$ is the unknown electric surface current, $\nabla_{\Gamma}\cdot$ is the surface divergence on Γ , and \mathcal{S} is the single layer potential operator

$$(\mathcal{S}\mathbf{J})(\mathbf{r}) = \int_{\Gamma} G(\mathbf{r} - \mathbf{r}')\mathbf{J}(\mathbf{r}') d\sigma_{r'}. \quad (2)$$

The Green's function $G(\mathbf{r}) = e^{ik|\mathbf{r}|}/(4\pi|\mathbf{r}|)$ is the fundamental solution to the Helmholtz equation with the free space wave number $k = \omega\sqrt{\epsilon\mu}$, where ϵ and μ are the permittivity and permeability of the medium where the antenna is embedded in.

The state problem (1) is discretized using the method of moments (MoM) which is the Galerkin method applied to (1). Let $V(\Gamma)$ be a space of vector-valued functions spanned by basis functions $\boldsymbol{\psi}_n$, $n = 1, \dots, N$ defined on the triangulated surface Γ .

The approximate state problem then reads as follows:

$$\text{Find } \mathbf{J} \in V(\Gamma) : \quad a_\Gamma(\mathbf{u}, \mathbf{J}) = b_\Gamma(\mathbf{u}) \quad \forall \mathbf{u} \in V(\Gamma). \quad (3)$$

Here the bilinear form $a_\Gamma(\cdot, \cdot)$ and the linear form $b_\Gamma(\cdot)$ are given by

$$\begin{aligned} a_\Gamma(\mathbf{u}, \mathbf{J}) &= -i\omega\mu \int_\Gamma \mathbf{u}(\mathbf{r}) \cdot (\mathcal{S}\mathbf{J})(\mathbf{r}) d\sigma - \frac{1}{i\omega\epsilon} \int_\Gamma \nabla_\Gamma \cdot \mathbf{u}(\mathbf{r})(\mathcal{S}\nabla_\Gamma \cdot \mathbf{J})(\mathbf{r}) d\sigma \\ b_\Gamma(\mathbf{u}) &= \int_\Gamma \mathbf{u} \cdot \mathbf{E}^p d\sigma. \end{aligned}$$

To construct $V(\Gamma)$ we utilize Rao–Wilton–Glisson (RWG) [5] functions without edge length scaling. Those functions are surface-divergence conforming and omitting the edge length scaling makes them coincide with the lowest order Raviart–Thomas basis functions. Denoting the RWG basis functions with $\boldsymbol{\psi}^n$, $n = 1, \dots, N$, the problem (3) has an algebraic representation

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad (4)$$

where the entries of the matrix \mathbf{A} and the excitation vector \mathbf{b} are given by $A_{mn} = a_\Gamma(\boldsymbol{\psi}^m, \boldsymbol{\psi}^n)$ and $b_m = b_\Gamma(\boldsymbol{\psi}^m)$.

3 ALGEBRAIC SHAPE SENSITIVITY ANALYSIS

In this section we describe a generic framework for shape derivatives of objective functions that depend on the shape and the surface current solution of the scatterer. See [6, 7, 3] for further details.

Let us suppose that Γ is a surface tessellated with planar triangles whose vertices are denoted by $(\mathbf{p}_l)_{l=1}^L$. Let $\boldsymbol{\alpha} \in \mathbb{R}^M$ be a vector of parameters and $(\boldsymbol{\phi}_m)_{m=1}^M$ be a family of functions so that $F_\alpha : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, $F_\alpha(\mathbf{r}) = \mathbf{r} + \sum_m \alpha_m \boldsymbol{\phi}_m(\mathbf{r})$ is a sufficiently smooth map whenever $|\boldsymbol{\alpha}|$ is small enough. We can now identify a deformed configuration of Γ , namely $\Gamma_\alpha = F_\alpha(\Gamma)$, with the parameter vector $\boldsymbol{\alpha}$. Note that F_α need not to be linear with respect to $\boldsymbol{\alpha}$ as for the sensitivity analysis only the linearized mapping is needed.

We consider linear combination of deformation maps that are obtained by varying the vertices of the original triangulated surface, i.e. $\boldsymbol{\phi}_m(\mathbf{r}) = \sum_{l=1}^L \boldsymbol{\tau}_{lm} \lambda_l(\mathbf{r})$, where λ_l are the piecewise linear and continuous functions satisfying $\lambda_l(\mathbf{p}_k) = \delta_{lk}$.

Let a real valued objective functional $J : \mathbb{R}^M \times \mathbb{C}^N \rightarrow \mathbb{R} : (\boldsymbol{\alpha}, \mathbf{x}) \mapsto J(\boldsymbol{\alpha}, \mathbf{x})$ depending on the shape-parameters $\boldsymbol{\alpha}$ and the degrees of freedom of the discrete surface current $\mathbf{J}_\alpha = \sum_n x^n \boldsymbol{\psi}^n$ be given. In practical applications it is common that \mathbf{b} does not depend on $\boldsymbol{\alpha}$, e.g., when the system is excited with the voltage-gap feed and the geometry around the feed port remains unchanged. Thus, we restrict to the following abstract optimization problem:

$$\underset{\boldsymbol{\alpha} \in \mathbb{R}^M, \mathbf{x}_\alpha \in \mathbb{C}^N}{\text{minimize}} \quad J(\boldsymbol{\alpha}, \mathbf{x}_\alpha) \quad (5)$$

subject to

$$\mathbf{A}_\alpha \mathbf{x}_\alpha = \mathbf{b}. \quad (6)$$

Employing the classical adjoint variable method [6] we find that the derivatives $\frac{d}{d\alpha_m} J$ are given by

$$\frac{dJ}{d\alpha_m} = \frac{\partial J}{\partial \alpha_m} - \Re \left\{ \gamma^\top \frac{\partial \mathbf{A}_\alpha}{\partial \alpha_m} \mathbf{x}_\alpha \right\} \quad (7)$$

where γ is the solution of the adjoint equation

$$\mathbf{A}_\alpha \gamma = \overline{\nabla_x J}. \quad (8)$$

Above we have used the fact that from the symmetry of $a_\Gamma(\cdot, \cdot)$ it follows that the system matrix is symmetric (but not Hermitian), i.e. $\mathbf{A}_\alpha^\top = \mathbf{A}_\alpha$. The complex gradient $\nabla_x J$ is defined by $\nabla_x J = (\nabla_{\Re \mathbf{x}} + i \nabla_{\Im \mathbf{x}}) J$, where the operators $\nabla_{\Re \mathbf{x}}$ and $\nabla_{\Im \mathbf{x}}$ are the gradients with respect to real and imaginary part of \mathbf{x} , respectively.

Looking at equations (7)–(8) we find that in order to compute the gradient of J with respect to the shape-parameters, one needs to compute the partial derivatives $\frac{\partial}{\partial \alpha_m} J$, the matrix-vector products with the differentiated system matrix $\frac{\partial \mathbf{A}_\alpha}{\partial \alpha_m} \mathbf{x}_\alpha$, the solution vector \mathbf{x}_α , and the solution γ of the adjoint equation. The system matrices of the state and the adjoint equations are identical. Thus no new solver needs to be implemented to solve the adjoint equation (8). The derivatives $\frac{\partial \mathbf{A}_\alpha}{\partial \alpha_m}$ can be computed analytically [4], with a difference formula or with automatic differentiation [3, 8].

The drawback, however, of MoM-EFIE formulation for the Maxwell system is that the coefficient matrix \mathbf{A} is a full matrix. This is opposite to e.g., the finite element case where the matrix is sparse. The time and storage complexity to solve equations (6), (8) is $\mathcal{O}(N^3)$ and $\mathcal{O}(N^2)$, respectively. Also the time complexity of the evaluation of the last term in (7) is $\mathcal{O}(N^2)$.

For the simulation and optimization of electromagnetically large objects, one needs to employ more advanced method as the multilevel fast multipole method. In the next section we will shortly describe the idea of MLFMA and show how the sensitivity analysis can be augmented to any existing MLFMA implementation.

4 FAST MATRIX-VECTOR PRODUCT AND ITS GEOMETRIC SENSITIVITY

Instead of applying standard Gaussian elimination to the (possibly very large) linear system (6), we consider iterative Krylov subspace methods like GMRES. Instead of manipulating stored matrix elements, Krylov subspace methods only need results of matrix-vector products, i.e. given a vector \mathbf{z} , compute $\mathbf{y} = \mathbf{A}\mathbf{z}$. Of course, in order to be of practical interest, either the number of iterations (i.e. the number of matrix-vector products) and/or the cost of a matrix-vector product must be sufficiently small.

The idea of MLFMA is the fast evaluation of the matrix product $\mathbf{y} = \mathbf{A}\mathbf{z}$. It is based on the division of the matrix into “near” and “far” terms,

$$\mathbf{A} = \mathbf{A}_{near} + \mathbf{A}_{far}. \quad (9)$$

The entries A_{near}^{pq} of the sparse matrix \mathbf{A}_{near} dealing with near interactions is evaluated in the standard way and stored. The entries A_{far}^{pq} corresponding to far interactions are evaluated approximately but not stored.

The MLFMA applied to EFIE is based on the following approximation [9, 10]. Let us consider the computation of the far terms A_{far}^{pq} in (9). Let Q_1 and Q_2 be two cubes such that

$\text{supp}(\psi^p) \subset Q_1$, $\text{supp}(\psi^q) \subset Q_2$, and the distance \mathbf{D} of the centers of Q_1 and Q_2 is large enough. We make the following approximation

$$A_{far}^{pq} = a_{\Gamma}(\psi^p, \psi^q) \approx ik \int_{\Gamma} \psi^p(\mathbf{r}) \cdot \int_{S^2} e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}} \mathbf{F}_{\psi^q}^{\infty}(\hat{\mathbf{k}}) T_L(\mathbf{D}, \hat{\mathbf{k}}) d\hat{\mathbf{k}} d\sigma_{\mathbf{r}}, \quad (10)$$

which can be made arbitrarily good by taking $L \rightarrow \infty$. Here $\hat{\mathbf{k}} = (\cos \phi \sin \theta, \sin \phi \cos \theta, \cos \theta)$, $\phi \in [0, 2\pi]$, $\theta \in [0, \pi]$, $\int_{S^2} d\hat{\mathbf{k}}$ denotes the integration over the surface of a three-dimensional unit ball,

$$\mathbf{F}_{\Phi}^{\infty}(\hat{\mathbf{k}}) = \frac{-k}{\omega \varepsilon_0} \int_{\Gamma} e^{-ik\hat{\mathbf{k}} \cdot \mathbf{r}'} \hat{\mathbf{k}} \times \hat{\mathbf{k}} \times \Phi(\mathbf{r}') d\sigma_{\mathbf{r}'}. \quad (11)$$

is the far-field pattern from the surface current Φ , and

$$T_L(\mathbf{D}, \hat{\mathbf{k}}) = \frac{ik}{4\pi} \sum_{n=0}^L i^n (2n+1) h_n^{(1)}(k|\mathbf{D}|) P_n \left(\frac{\mathbf{D}}{|\mathbf{D}|} \cdot \hat{\mathbf{k}} \right), \quad (12)$$

is the Rokhlin translation function [11] given in terms of spherical Hankel functions $h_n^{(1)}$ and Legendre polynomials P_n .

The matrix \mathbf{A}_{near} is a sparse one and the product $\mathbf{A}_{near} \mathbf{z}$ can be evaluated in $\mathcal{O}(N)$ time. Now, organizing the computations for A_{far}^{pq} in a hierarchical way, one can obtain an $\mathcal{O}(N \log^2 N)$ algorithm to compute $\mathbf{A}_{far} \mathbf{z}$. We refer to [9, 10, 12] for the algorithmic details.

As seen from (7), it is not mandatory to construct the differentiated system matrices $\frac{\partial \mathbf{A}_{\alpha}}{\partial \alpha_m}$ to obtain sensitivities of \mathcal{J} . Instead, it suffices to calculate the matrix-vector products $\frac{\partial \mathbf{A}_{\alpha}}{\partial \alpha_m} \mathbf{x}_{\alpha}$. It should be also noted that the derivatives of the near field interactions parts of the system matrix $\partial[\mathbf{A}^{near} \mathbf{x}_{\alpha}]/\partial \alpha_m$ can be computed in the assembly loop in the usual element by element manner as discussed in [4].

Rewriting the formula for the far interactions (10) in the perturbed geometry Γ_{α}

$$a_{\Gamma_{\alpha}}(\psi_{\alpha}^p, \psi_{\alpha}^q) \approx -\frac{ik^2}{\omega \varepsilon} \int_{S^2} T_L(\mathbf{D}, \hat{\mathbf{k}}) \int_{\Gamma_{\alpha}} \psi_{\alpha}^p(\mathbf{r}) e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}} \cdot \int_{\Gamma_{\alpha}} e^{-ik\hat{\mathbf{k}} \cdot \mathbf{r}'} \hat{\mathbf{k}} \times \hat{\mathbf{k}} \times \psi_{\alpha}^q(\mathbf{r}') d\sigma_{\mathbf{r}'} d\sigma_{\mathbf{r}} d\hat{\mathbf{k}}, \quad (13)$$

we see that only aggregation and disaggregation (i.e. integrations with respect to \mathbf{r} and \mathbf{r}') depend upon small perturbations of the geometry. Thus, in order to compute the approximations of the derivatives $\partial a_{\Gamma_{\alpha}}(\psi_{\alpha}^p, \psi_{\alpha}^q)/\partial \alpha_m$ we need to differentiate the expressions

$$I_1(\psi_{\alpha}^p, \Gamma_{\alpha}) := \int_{\Gamma_{\alpha}} \psi_{\alpha}^p(\mathbf{r}) e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}} d\sigma_{\mathbf{r}} \quad \text{and} \quad I_2(\psi_{\alpha}^q, \Gamma_{\alpha}) := \int_{\Gamma_{\alpha}} \hat{\mathbf{k}} \times \hat{\mathbf{k}} \times \psi_{\alpha}^q(\mathbf{r}') e^{-ik\hat{\mathbf{k}} \cdot \mathbf{r}'} d\sigma_{\mathbf{r}'}. \quad (14)$$

The derivatives $\frac{\partial I_1}{\partial \alpha_m}$ and $\frac{\partial I_2}{\partial \alpha_m}$ can be evaluated with any method that gives the desired accuracy, but due to simplicity of the above formulas we consider the change of variables approach taken in [4] and calculate the derivatives analytically.

The derivatives are evaluated analytically by representing the basis functions on Γ_{α} as mapped basis functions of Γ . To that end we utilize the contravariant Piola transformation that reads

$$\psi^p \mapsto \frac{1}{\det F'_{\alpha}} F'_{\alpha} \psi^p \circ F_{\alpha}^{-1}. \quad (15)$$

It holds that this mapping tends to identity as $\alpha \rightarrow 0$ and that it is bijective as $V(\Gamma) \rightarrow V(\Gamma_{\alpha})$. Thus, for each RWG function ψ_{α}^p there is such an RWG function ψ^p that

$$\psi_{\alpha}^p = \frac{1}{\det F'_{\alpha}} F'_{\alpha} \psi^p \circ F_{\alpha}^{-1}. \quad (16)$$

Here F'_α is the jacobian matrix of F_α given by

$$F'_\alpha(\mathbf{r}) = \mathbf{I} + \sum_m \alpha_m \sum_l \boldsymbol{\tau}_{lm} (\nabla_\Gamma \lambda_l(\mathbf{r}))^T. \quad (17)$$

As $\nabla_\Gamma \lambda_l$ is piecewise constant, the matrix function F'_α is piecewise constant too.

Performing the change of variables we get

$$\int_{\Gamma_\alpha} \boldsymbol{\psi}_\alpha^p(\mathbf{r}) e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}} d\sigma_r = \int_\Gamma \frac{F'_\alpha(\mathbf{r}) \boldsymbol{\psi}^p(\mathbf{r})}{\det F'_\alpha} e^{ik\hat{\mathbf{k}} \cdot F_\alpha(\mathbf{r})} \det F'_\alpha d\sigma_r. \quad (18)$$

Note that the determinant $\det F'_\alpha$ cancels out in (18).

Finally, the derivative of I_1 is given by

$$\begin{aligned} \left. \frac{\partial I_1}{\partial \alpha_m} \right|_{\alpha_m=0} &= \int_\Gamma \frac{\partial}{\partial \alpha_m} \left[F'_\alpha(\mathbf{r}) \boldsymbol{\psi}^p(\mathbf{r}) e^{ik\hat{\mathbf{k}} \cdot F_\alpha(\mathbf{r})} \right]_{\alpha_m=0} d\sigma_r \\ &= \sum_l \int_\Gamma \left[\boldsymbol{\tau}_{lm} \nabla_\Gamma \lambda_l(\mathbf{r}) \cdot \boldsymbol{\psi}^p(\mathbf{r}) + \boldsymbol{\psi}^p(\mathbf{r}) \lambda_l(\mathbf{r}) ik\hat{\mathbf{k}} \cdot \boldsymbol{\tau}_{lm} \right] e^{ik\hat{\mathbf{k}} \cdot \mathbf{r}} d\sigma_r. \end{aligned} \quad (19)$$

Similarly,

$$\left. \frac{\partial I_2}{\partial \alpha_m} \right|_{\alpha_m=0} = \sum_l \int_\Gamma \hat{\mathbf{k}} \times \hat{\mathbf{k}} \times \left[\boldsymbol{\tau}_{lm} \nabla_\Gamma \lambda_l(\mathbf{r}) \cdot \boldsymbol{\psi}^q(\mathbf{r}) + \boldsymbol{\psi}^q(\mathbf{r}) \lambda_l(\mathbf{r}) ik\hat{\mathbf{k}} \cdot \boldsymbol{\tau}_{lm} \right] e^{-ik\hat{\mathbf{k}} \cdot \mathbf{r}} d\sigma_r \quad (20)$$

Applying the product rule of differentiation to (13) we see that instead of just taking the ϕ and θ components of the far field pattern arising from $\boldsymbol{\psi}^q$ through the MLFMA procedure, also for the expression $\left. \frac{\partial I_2}{\partial \alpha_m} \right|_{\alpha_m=0}$ the far-field pattern must be computed and translated. However, the action of the differentiated system matrix needs to be calculated only once per shape-parameter. Thus, the extra work is negligible when considering shape optimization problems where the state equation is solved iteratively.

The time spent in the MLFMA accelerated part of the matrix vector product is small compared to the solution time of the state equation and the adjoint equation and, furthermore, it scales as $O(K \log^2 K)$, where K is the number of edges which undergo geometric perturbation.

For more details and a numerical example, we refer to [13].

5 CONCLUSION

We considered an efficient approach to accelerate the matrix-vector product involving shape differentiated system matrix with the fast multipole method. We showed that the analytical (algebraic) sensitivity analysis can be done efficiently despite the fact that the full system matrix is defined only implicitly.

Using this approach, adding algebraic sensitivity analysis capability to simulation code requires some relatively minor changes in the code. In the MLFMA part, only the start and the end of aggregation-translation-disaggregation process must be modified and for the near interaction the routine that computes element pair interactions must be modified. Furthermore, a perturbation vector for each vertex of the mesh and shape-parameter must be provided for the solver.

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