Singular Analytical Integration for Efficient Volume Integral Equation Implementation

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Abstract— We present a novel efficient implementation of the Volume Integral Equation formulation, for the analysis of printed circuits with finite size dielectric objects. The singularity of the Green’s functions is extracted from the kernel of the integral equation, as static terms. These terms are then evaluated analytically for coincident rectangular cells in two and three dimensions. A semi-analytical formulation is also derived for the interactions involving adjacent cells. Results show the gain in efficiency and accuracy that can be obtained in the frame of the Volume Integral Equation formulation, when the new analytical techniques are used.

1. INTRODUCTION

The Volume Integral Equation technique (VIE) is a widely used formulation for the analysis of a large class of problems containing dielectric objects of finite dimensions and complex shapes. In this type of problems, Green’s functions can not account for the dielectric objects in a semi-analytic fashion, and one has to resort to the use of the well known free-space Green’s functions. With this formulation the dielectric objects are modeled with the aid of polarization currents defined on their volumes. The subsequent application of the Method of Moments (MoM) requires the computation of overlapping integrals between the free space Green’s functions and the basis and testing functions. An interesting feature when developing this approach, is that surface charge distributions appear at the outer surfaces of homogeneous bodies. As a result, several combinations of surface and volume integrals need to be computed, before filling up the complete MoM matrix system. The whole situation is even more complicated, due to the singular behavior of the Green’s functions used inside the Kernel of the integral equations.

In the above frame, the authors have derived an efficient implementation of the Volume Integral Equation (VIE) approach, by following different singularity extraction techniques, combined with analytical integration. First, a Taylor series expansion is applied to the free-space Green’s functions, splitting the whole contribution in static and dynamic parts. The dynamic part thus obtained is not anymore singular, and it can be integrated numerically without effort. What remains, then, is the calculation of the static terms, containing the singular behavior of the Kernel. Now, the main difficulty in the implementation of this formulation is the integration of coincident basis and testing cells for these static terms. This is because of the well known singularity of the potential Green’s functions. To overcome this problem, integration techniques based on polar and spherical coordinates have been developed in the past [1].

In this paper, we propose to apply analytical integration to these singular terms. The analytical integration increases accuracy, and reduces considerably the computational cost. The analytical integration is based on the dyadic identities reported in [2], which are extended for the first time to account for volume integration, and mixed surface-volume interactions, in rectangular and hexahedral domains. Besides, the authors have also treated for the first time the quasi-singular case of adjacent cells. For these adjacent cells, the fast variations due to the quasi-singular behavior of the kernel may introduce important errors during numerical integration. To overcome this problem, we propose in this paper to evaluate analytically the source contribution of the integrals for this quasi-singular situation.

The included results show the efficiency and accuracy of the new approach for the treatment of the singularity, in comparison with direct numerical integration. The presented results show big improvements in efficiency and accuracy during the analysis of practical devices using the VIE approach.
2. THEORY

The formulation under consideration is a general VIE technique including metallic and dielectric objects [3]. First, the static terms of the Green’s functions are extracted following a Taylor series expansion [4]. A standard VIE formulation leads to the following volume and surface integrals for the static terms:

\[ I_1 = \int_S \int_{S'} \frac{1}{R_S} dS' dS \quad \text{On metallic surfaces} \]  
\[ I_2 = \int_S \int_{S'} \frac{1}{R_S} \tilde{f}_b dS' dS \quad \text{On metallic surfaces} \]  
\[ I_3 = \int_V \int_{V'} \frac{1}{R_V} dV' dV \quad \text{In dielectric objects} \]  
\[ I_4 = \int_V \int_{V'} \frac{1}{R_V} \tilde{f}_b dV' dV \quad \text{In dielectric objects} \]  
\[ I_5 = \int_V \int_{S'} \frac{1}{R_V} dS' dV \quad \text{On the surfaces of dielectric objects} \]

where \( \tilde{f}_b \) and \( \tilde{f}_t \) are the basis and testing functions employed in the MoM implementation. Also, \( R_S \) is the spatial distance between observation and source points, considering two dimensions (surface case), whereas \( R_V \) is the volumetric counterpart of this distance. Integrals (1) and (3) are those corresponding to the static MoM contributions of the electric scalar potential in two and three dimensions, respectively. On the other hand, (2) and (4) refer to the contributions of the magnetic vector potential in the same cases. Finally, (5) corresponds to a mixed surface-volume interaction due to the external charges distributed in the outer surfaces of homogeneous bodies.

Integrals \( I_1 \) to \( I_5 \) can be performed numerically using standard quadrature rules, when source and observation integration domains do not coincide. For the coincident cases \( S = S' \) and \( V = V' \), a different strategy must be adopted in order to avoid numerical problems and serious inaccuracies. A useful approach consists in transforming the source and observation points into polar coordinates. It is well known that these transformations mathematically cancel the term \((1/R)\). The main disadvantage of this method is that many integration points must be considered to assure convergence in the numerical integrals.

To overcome this problem, a new strategy is proposed in this paper, based on the analytical integration of terms of the form \((1/R)\), for coincident surface and volume domains. The procedure for triangular surfaces was presented in [2]. Based on this work, the authors have adapted the procedure to rectangular domains, for both surface and volume cases (as illustrated in Fig. 1).

![General geometry of the integration domains considered in this paper.](image)

2.1. Identities and Integrals for Rectangular Domains

In [2], the authors started from a set of useful algebraic identities which helped to reduce the complexity of the MoM integrals. In two dimensions, and for rectangular surfaces, these identities
have the form:

\[
\frac{1}{R_S} = -\nabla_S \cdot \nabla'_S R_S \tag{6}
\]

\[
\frac{I}{R_S} = \nabla_S \times \nabla'_S \times \vec{f}_b - \nabla_S \cdot \nabla'_S R_S \tag{7}
\]

\[
\left( \nabla_S \times \vec{f}_b \right) = \nabla'_S \times \left( R_S \cdot \vec{f}_b \right) \tag{8}
\]

\[
\vec{f}_t \cdot \left( \nabla_S \nabla'_S R_S \right) = \nabla_S \cdot \left( \nabla'_S \cdot R_S \left[ \vec{f}_t \vec{f}_b + \frac{1}{3} \left( \vec{f}_t \vec{R}_S - \vec{R}_S \vec{f}_b \right) - \frac{1}{9} I \vec{R}_S^2 \right] \right) \tag{9}
\]

Here, the subscript \( S \) indicates that the spatial distance and the differential operators are expressed in two-dimensional coordinates (case of Fig. 1(a)). These are the same expressions that appear in [2] for triangular domains, except for the case of (9), where the constants \( \frac{1}{3} \) and \( \frac{1}{9} \) change depending on the definition of the basis functions employed (rectangular for our case).

These identities can now be extended to the 3D case of tetrahedral cells, resulting into:

\[
\frac{2}{R_V} = -\nabla_V \cdot \nabla'_V R_V \tag{10}
\]

\[
\frac{2I}{R_V} = \nabla_V \times \nabla'_V \times \vec{f}_b - \nabla_V \cdot \nabla'_V R_V \tag{11}
\]

\[
\left( \nabla'_V \times \vec{f}_b \right) = \nabla'_V \times \left( R_V \cdot \vec{f}_b \right) \tag{12}
\]

\[
\vec{f}_t \cdot \left( \nabla_V \nabla'_V R_V \right) = \nabla_V \cdot \left( \nabla'_V \cdot R_V \left[ \vec{f}_t \vec{f}_b + \frac{1}{4} \left( \vec{f}_t \vec{R}_S - \vec{R}_S \vec{f}_b \right) - \frac{1}{12} I \vec{R}_V^2 \right] \right) \tag{13}
\]

Now, the subscript \( V \) denotes that operations are performed in three dimensions (Fig. 1(b)). It can be noticed that these new identities maintain the same form as the previous ones, differing only in some constants that appear due to the additional spatial dimension. Finally, because we are also interested in mixed surface-volume interactions, an additional identity must be added to complete the whole set, namely:

\[
\frac{2}{R_V} = -\nabla_S \cdot \nabla'_S R_V + \frac{\partial^2}{\partial z^2} R_V \tag{14}
\]

Using these identities, in combination with the well known Gauss, Stokes and Curl theorems, the integrals expressed in (1) to (5) can be transformed into:

\[
I_1 = - \int_C \int_{C'} R_S \vec{u} \vec{u}' dl' dl \tag{15}
\]

\[
I_2 = - \int_C \int_{C'} R_S \vec{u} \left[ \vec{f}_t \vec{f}_b - \vec{f}_b \vec{f}_t + \frac{1}{3} \left( \vec{f}_t \vec{R}_S - \vec{R}_S \vec{f}_b \right) + I \left( \vec{f}_t \cdot \vec{f}_b - \frac{1}{9} R_S \right) \right] \vec{u}' dl' dl \tag{16}
\]

\[
I_3 = - \frac{1}{2} \int_S \int_{S'} R_V \vec{u} \vec{u}' dS' dS \tag{17}
\]

\[
I_4 = - \frac{1}{2} \int_S \int_{S'} R_V \vec{u} \left[ \vec{f}_t \vec{f}_b - \vec{f}_b \vec{f}_t + \frac{1}{4} \left( \vec{f}_t \vec{R}_S - \vec{R}_S \vec{f}_b \right) + I \left( \vec{f}_t \cdot \vec{f}_b - \frac{1}{12} R_V \right) \right] \vec{u}' dl' dS \tag{18}
\]

\[
I_5 = \frac{1}{2} \left( - \int_0^c \int_S \int_{S'} R_V \vec{u} \vec{u}' dS' dS + \int_S \int_{S'} \frac{c}{R_V |z - z'|} dS' dS \right) \tag{19}
\]

In above expressions, \( C \) and \( C' \) denote the linear contours of the integration cells, and the vectors \( \vec{u}, \vec{u}' \) are the outward vectors normal to the observation and source integration domains (linear or surface depending on the case), respectively. It is interesting to note that, due to the application of the identities, the term \( 1/R \) has changed to \( R \), which is not singular for \( R \to 0 \). Also, the complexity of the integration domains have been reduced in one dimension for each case. Hence, it is possible to evaluate analytically the expressions (15) to (18). Although the integration domains are simple, the final analytical results for all the integrals require very long
calculus and algebraic manipulations, specially in the case of the volumetric cells. These expressions are composed of simple logarithmic and inverse of trigonometric functions, depending only on the size cell dimensions. They can be evaluated, therefore, very fast with a computer. They are not included here for the sake of space.

Apart from the singularity cases already explained, other important sources of numerical errors are the MoM interactions between very close surface cells. Specially in the cases of adjacent cells (one or two common nodes), the numerical techniques applied to (1) and (2) do not behave properly, due to the fast variations of the Kernel for small source-observer distances. In order to minimize this effect, we propose to evaluate this kind of interactions following a semi-analytical procedure. The strategy consists in computing analytically the source contribution of $I_1$ and $I_2$, while the integral extended to the observer cell is computed numerically. The analytical integration on the source cell effectively eliminates the fast variations of the integral equation Kernel. Consequently, the numerical integration on the observer cell converges very fast.

3. RESULTS

In this section we will show the advantages and improvements of the new proposed approach. The calculation of the integrals has been performed for the MoM analysis of a practical microstrip device following the VIE formulation. The geometry under consideration is a metallic strip line of dimensions $0.8 \times 40 \text{ mm}$ printed over a $1 \text{ mm}$ substrate of alumina ($\varepsilon_r = 9.8$), and shielded in a metallic box of dimensions $40 \times 40 \times 4 \text{ mm}$.

We present in Fig. 2 the error obtained for the volume interactions computed numerically with the transformation to spherical coordinates, as compared to the closed-form solution obtained with the analytical expressions derived in this work. It can be noticed in the figure that errors below $10^{-3}$ are obtained when more than $10^3$ points are used in the numerical integration. When $14^3$ points are used, the total static MoM matrix needs 7.2 minutes to be computed, whereas only 17.1 seconds are needed when using the proposed analytical approach. This shows the bottleneck problem of the numerical method, when computing the singular interactions with high accuracy.

![Figure 2: Relative error between numerical and analytical values of $I_3$ as a function of the number of quadrature integration points.](image)

Now, we will examine the behavior of the semi-analytical approach for adjacent interactions. In Fig. 3, the efficiency of this new approach is compared to a standard numerical quadrature integration. First, Fig. 3(a) shows the relative errors obtained between the numerical and the semi-analytical values of $I_1$ and $I_2$, as a function of the distance between the centers of the source and observation cells. The number of quadrature points employed in the two methods has been optimized according to this distance. It can be observed that, as the distance decreases, the relative error grows, until significant values are obtained for the case of two adjacent cells (the first three points in the graphic). The discontinuity peaks that appear in the curves occur when the observation cell changes from one row to another row inside the mesh structure. As it can be noticed, the error is larger for the $I_2$ integral, where the linear variations of the basis functions are present. This is because these linear variations contribute to increase the fast variations of the Kernel for small source-observer distances.
On the other hand, Fig. 3(b) shows the effects of the number of quadrature points employed in the evaluation of the integrals using the two methods (pure numerical and semi-analytical). For this test we have considered the most critical case of two adjacent cells. The relative errors are taken with respect to the value obtained with a sufficiently large number of quadrature points (60) for all cases. It is interesting to observe how the analytical integration of the source contribution in $I_1$ allows to reduce the error several orders of magnitude with respect to the standard case of the double numerical integration. This fact helps to efficiently reduce the maximum number of quadrature points, and still achieve high accuracy.

![Figure 3: Comparison of numerical and semi-analytical approaches for the calculation of $I_1$ and $I_2$. Sizes of the cells are $a = 0.4$ mm, $b = 2.66$ mm, (a) Relative error as a function of the distance between cells, (b) Relative error as a function of the number of quadrature integration points.](image)

4. CONCLUSIONS

In this paper we have presented a new efficient technique for evaluating the singular contributions in the general frame of a volume integral equation (VIE) formulation solved by MoM. First, the singular behavior is extracted from the free space Green’s functions, and it is isolated in static terms for the vector and scalar potentials. A novel analytical integration in rectangular domains is then applied to these static terms. It is shown that the new technique improves the accuracy and reduces the computational cost, as compared to pure numerical integration. Also, the quasi-singular case of adjacent cells has been evaluated semi-analytically, reducing in this way the errors introduced by standard numerical integration. Useful numerical results are presented to confirm the practical value of the new approach.

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