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A COMPLETE VARIATIONAL METHOD FOR CAPACITANCE EXTRACTIONS

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Abstract—In the past, coupling capacitances between conductors was extracted using charge distributions directly. In this paper a set of new generalized variational formulas are derived. They are complete since they are valid not only for self-capacitances, but also for mutual capacitances. As for the realistic numerical implementation, elastance matrices become asymmetrical because of numerical method used. Then a more general variational formula is derived to account for the asymmetrical elastance matrix case. By these novel formulas the computational accuracy can be significantly improved compared to the conventional capacitance extraction method.

1. INTRODUCTION

Finding the capacitance of a metallic structure has been a problem of historical interest. The capacitance of a sphere can be easily found in closed form, while the closed-form capacitance of two spheres can be found by the image method [1]. When the object is of odd shape, usually no closed-form solution exists. For two-dimensional problems, the conformal mapping method can be used to solve Laplace's equation, and hence yielding the capacitance of complex two-dimensional structures [2].

When the structure is three dimensional, finding analytic solution is even more difficult. Kirchhoff first gave the asymptotic formula for the capacitance of two circular discs with small separation in 1877 [3]. Since then, formulas for the capacitance of this structure has been derived by others [4–8].

When microwave integrated circuits became important, it was then useful to find the capacitance of two circular disks separated by a dielectric slab [9–14]. This geometry is encountered in the microstrip capacitance which forms an important component of microwave integrated circuits.

Recently, the increasing clock frequency of computer chip design has rekindled the interest in capacitance extraction of complex structures as found in computer chips. The mutual capacitive coupling between conductors causes cross-talk that can degrade the performance of high-speed circuits. Hence, capacitance extraction, and the understanding of cross-talk effect have been an important part of these circuit designs.

When the wavelength is very long compared to the circuit size, Laplace's equation can be solved to obtain the mutual capacitance between conductors. Because of complex circuit structures for which no closed form exists, and the large number of unknowns needed to model these complex structures, computational electromagnetics (CEM) with fast algorithms have been widely used to solve these problems [15–21].

A traditional way to extract capacitances is to discretize the conductors into small patches and use the Galerkin's method or the method of moments (MoM) to solve for the charge distribution from a resultant linear system. The mutual and self-capacitances can then be obtained from them directly [1, 22, 23].

The most popular way to model coupling capacitances was to use the elastance matrix [1]. Consider N initially uncharged conductors of fixed positions and shapes. The ratio of the rise in potential V_r of conductor r due to the charge Q_s placed on conductor s (with zero charges on all other conductors) to produce this rise is called the coefficient of potential or mutual elastance s_{rs}. A superposition of potentials for charges over all conductors gives

$$\begin{aligned} V_1 &= s_{11}Q_1 + s_{12}Q_2 + \cdots + s_{1N}Q_N \\ V_2 &= s_{21}Q_1 + s_{22}Q_2 + \cdots + s_{2N}Q_N \\ \cdots &= \cdots \\ V_N &= s_{N1}Q_1 + s_{N2}Q_2 + \cdots + s_{NN}Q_N \end{aligned} \tag{1}$$

Once the elastance matrix is known, we may solve this set of equations to obtain the charge on each conductor in terms of the potentials of neighboring conductors. The solutions are

$$\begin{aligned} Q_1 &= c_{11}V_1 + c_{12}V_2 + \cdots + c_{1N}V_N \\ Q_2 &= c_{21}V_1 + c_{22}V_2 + \cdots + c_{2N}V_N \\ \cdots &= \cdots \\ Q_N &= c_{N1}V_1 + c_{N2}V_2 + \cdots + c_{NN}V_N \end{aligned} \tag{2}$$

The quantity c_{rr} is the self-capacitance, while c_{rs} is the mutual capacitance. The matrix formed by c_{ij} is known as the capacitance matrix. Suppose V_r is set to be a nonzero constant while all other conductors are grounded to zero potential. Then the elements of the capacitance matrix are simply written as

$$\begin{aligned} c_{1r} &= Q_1^r/V_r \\ c_{2r} &= Q_2^r/V_r \\ \cdots &= \cdots \\ c_{Nr} &= Q_N^r/V_r \end{aligned} \tag{3}$$

where Q_s^r refers to the net charge on the sth conductor while the rth conductor is set to a nonzero voltage V_r.

Usually, Q_s^r cannot be exactly determined, and is sought by some approximate numerical method. For the self-capacitance, there is a variational formula that can improve its accuracy compared to the method using Equation (3). It states that under the above assumption, the self-capacitance is written as the variational formula [24, p. 53], [25, p. 277]

$$c_{rr}^{-1}[\sigma] = \frac{\oint_{s_r} dr \oint_{s_r} dr' \sigma(\mathbf{r}) G(\mathbf{r}, \mathbf{r}') \sigma(\mathbf{r}')}{\left[\oint_{s_r} dr \sigma(\mathbf{r})\right]^2} \tag{4}$$

where $\sigma(\mathbf{r})$ refers to the charge distribution on the rth conductor, $G(\mathbf{r}, \mathbf{r}')$ is the static Green's function, and s_r denotes the surface of the rth conductor. Reference [24] has stipulated this Green's function to be one that will produce the potential due to a point charge in the presence of all the conductors except for the rth conductor.

However, there is no variational formula for mutual capacitances. Hence, the variational method is not complete and has been rarely used for capacitance extractions. In this paper, new variational formulas for capacitance extractions are derived. They are complete because they are valid not only for self-capacitances but also for mutual capacitances. Furthermore, during numerical computations, an approximate matrix equation is usually derived by the projection method such as the Galerkin's method or the method of moments to solve for the capacitance matrix. The projection method may cause the elastance matrix to be asymmetrical. A formula for the asymmetric case is specially derived to give the variational property of the capacitance computation. They provide higher accuracy for the capacitance compared to the conventional method.

2. VARIATIONAL FORMULAS FOR CAPACITANCE EXTRACTIONS

The capacitance matrix is often obtained via a numerical procedure described below. Suppose that there are N conductors arbitrarily placed in an isotropic inhomogeneous medium environment. The pertinent integral equation is

$$\oint_s d\mathbf{r}' G(\mathbf{r}, \mathbf{r}')\sigma(\mathbf{r}') = V_i, \qquad \mathbf{r} \in s_i, \qquad i = 1, \cdots, N \tag{5}$$

where s_i is the surface of the ith conductor, $s = \cup_{i=1}^{N} s_i$, $\sigma(\mathbf{r}')$ is the surface charge density on all the conductors, and V_i is the potential of the ith conductor. The Green's function here is one that will produce the potential due to a point charge in the presence of an inhomogeneous medium (e.g., see reference [20]), and hence, is somewhat different from that defined in [24]. We can generalize the above to

$$\oint_s d\mathbf{r}' G(\mathbf{r}, \mathbf{r}')\sigma(\mathbf{r}') = \Phi(\mathbf{r}), \qquad \mathbf{r} \in s \tag{6}$$

A popular way to convert this integral equation into a matrix equation is to use Galerkin's method, or the method of weighted residuals, also known as the method of moments. To this end, we let

$$\sigma(\mathbf{r}) = \sum_{n=1}^{N} q_n f_n(\mathbf{r}) \tag{7}$$

where $f_n(\mathbf{r})$ is the basis function. Substituting the above into (6), and multiplying by $w_m(\mathbf{r})$ where $m = 1, \cdots, N$, and integrate over s, we have

$$\overline{\mathbf{S}} \cdot \mathbf{q} = \mathbf{\Phi} \tag{8}$$

where

$$[\overline{\mathbf{S}}]_{mn} = \oint_s d\mathbf{r} \oint_s d\mathbf{r}' w_m(\mathbf{r}) G(\mathbf{r}, \mathbf{r}') f_n(\mathbf{r}') \tag{9}$$

$$[\mathbf{q}]_n = q_n \tag{10}$$

$$[\mathbf{\Phi}]_m = \oint_s d\mathbf{r} w_m(\mathbf{r})\Phi(\mathbf{r}). \tag{11}$$

Since Laplace's equation is self-adjoint, the corresponding Green's function is also self-adjoint, and we expect the ensuing matrix equation via the above projection method to be symmetric. However, the

above represents a general nonsymmetric system unless $w_m = f_m$, the Galerkin's method case. When the basis functions $f_n(\mathbf{r})$ are normalized such that they hold unit charges, namely $\oint_s dr f_n(\mathbf{r}) = 1$, then q_n above represents the charge belonging to each basis function. Without loss of generality, we can also assume that $w_m(\mathbf{r})$ is similarly normalized.

Usually, to obtain an accurate solution and to provide versatility for geometry modeling, a subdomain method is used where the surfaces of all conductors are discretized into M small patches. One or more unknown functions is assigned to approximate the charge on each patch. The $\overline{\mathbf{S}}$ matrix above is the generalized elastance matrix whose value depends on the geometry, the Green's function, as well as the choice of expansion and weighting functions.

For capacitance computation, usually, the ith of the N conductors is set to a nonzero voltage V_i, while all the other conductors are set to zero volt. Hence, all patches that belong to the ith conductor will share the same potential V_i while the rest of the patches have zero volt. We denote such a matrix system as:

$$\overline{\mathbf{S}} \cdot \mathbf{q}^i = \mathbf{\Phi}^i \tag{12}$$

The vector $\mathbf{\Phi}^i$ is such that

$$[\mathbf{\Phi}^i]_m = \begin{cases} V_i, & \text{when support of } w_m \in s_i; \\ 0, & \text{when support of } w_m \notin s_i; \end{cases} \tag{13}$$

We can solve the above for q_n^i. For a given $\mathbf{q}^i$, by summing over q_n^i that belongs to the jth conductor to obtain the charge on it, namely, Q_j^i, we can use (3) to find the capacitance c_{ji} for $j = 1, \cdots, N$. Repeating this for $i = 1, \cdots, N$, we can find the self and mutual capacitances needed in (2) to obtain the capacitance matrix $\overline{\mathbf{C}}$ for which the following holds:

$$\overline{\mathbf{C}} \cdot \mathbf{V} = \mathbf{Q} \tag{14}$$

where $\mathbf{V}$ is the potential vector and $\mathbf{Q}$ is the charge vector of all conductors. The above relationship holds true for an arbitrary vector $\mathbf{V}$ as well. In the following discussion, we will specialize it to the case where only the ith element in $\mathbf{V}$ is nonzero.

The component Q_j^i of $\mathbf{Q}$ is defined as the net charge on the jth conductor while the ith conductor is assigned nonzero volt, and can be expressed as

$$Q_j^i = \sum_{n \in G_j} q_n^i \quad G_j = \{n : \text{support of } f_n \in s_j, \text{surface of } j\text{th conductor}\} \tag{15}$$

where $n = 1, 2, \cdots, M$ and $i, j = 1, 2, \cdots, N$. Since only the ith conductor is set to V_i and all others set to zero, it can be seen that

$$C_{ji} V_i = Q_j^i \tag{16}$$

This formula actually corresponds to the conventional direct capacitance computation method. It can be seen that the charge Q_j^i can be written in another form

$$Q_j^i = \frac{\mathbf{\Phi}^{j^t} \cdot \mathbf{q}^i}{V_j} \tag{17}$$

Putting Equation (12), (16) and (17) together, we get

$$C_{ji} = \frac{\mathbf{\Phi}^{j^t} \cdot \mathbf{q}^i}{V_i V_j} = \frac{\mathbf{\Phi}^{j^t} \cdot \overline{\mathbf{S}}^{-1} \cdot \mathbf{\Phi}^i}{V_i V_j} \tag{18}$$

Considering Equation (12) and assuming that Galerkin's method has been used to ensure the symmetry of $\overline{\mathbf{S}}$, we have

$$C_{ji}^{-1} = \frac{\mathbf{q}^{j^t} \cdot \overline{\mathbf{S}}^{-1} \cdot \mathbf{q}^i}{Q_j^i Q_i^j} \tag{19}$$

It can be seen that if $i = j$, Equation (19) changes into the self-capacitance formula similar but not identical to (4). The charge $\mathbf{q}^i$ in (19) represents the charge on all the conductors, whereas the charge in (4) represents the charge on the pertinent conductor only. When $i \neq j$, Equation (19) gives the mutual capacitance formula. Furthermore, it is a variational formula as shall be proven.

THEOREM 1 *The direct capacitance extraction method using Equation (16) is not variational. The formula in Equation (19) is variational.*

Proof It is obvious that Equation (16) is not stationary since the capacitance has the first order error caused by the charge error. As for the second statement, we take the first variation of Equation (19) about $\mathbf{q}^i$ and $\mathbf{q}^j$ which are exact solutions to (12). Then, we have

$$\delta C_{ji}^{-1} Q_j^i Q_i^j + C_{ji}^{-1} \delta Q_j^i Q_i^j + C_{ji}^{-1} Q_j^i \delta Q_i^j = \delta \mathbf{q}^{j^t} \cdot \overline{\mathbf{S}} \cdot \mathbf{q}^i + \mathbf{q}^{j^t} \cdot \overline{\mathbf{S}} \cdot \delta \mathbf{q}^i \tag{20}$$

From Equation (12), the right hand side (RHS) of the above equation is

$$RHS = \delta \mathbf{q}^{j^t} \cdot \mathbf{\Phi}^i + \mathbf{\Phi}^{j^t} \cdot \delta \mathbf{q}^i = \delta Q_i^j V_i + \delta Q_j^i V_j$$

From Equation (16), the left hand side (LHS) is

$$LHS = \delta C_{ji}^{-1} Q_j^i Q_i^j + V_j \delta Q_j^i + V_i \delta Q_i^j$$

Comparing both sides, it can be seen that $\delta C_{ji}^{-1} = 0$.

It is to be noted that if Equation (12) is solved exactly for $\mathbf{q}^i$ and $\mathbf{q}^j$, there is no difference between Equation (16) and Equation (19) to within machine precision of the exact computation. However, in many numerical computations, Equation (12) is not solved exactly. For example, it could have been solved by the conjugate gradient method or other iterative method for which a residual error in the solution remains. Alternatively, it could have been solved by some fast algorithms for which additional errors accrued due to the factorization of the Green's function. However, Equation (19) yields second order error in the capacitance when first order error is committed in the charge, and hence, is more accurate than Equation (16).

To arrive at the above result, we have assumed that Equation (12) is actually the equation constructed using Galerkin's method. Hence, the $\overline{\mathbf{S}}$ matrix is strictly symmetrical. Had the method of collocation or point matching method been used as in the method of weighted residuals, $\overline{\mathbf{S}}$ would have become asymmetrical. The asymmetry is caused by the choice of numerical methods. Then the important relation $\overline{\mathbf{S}} = \overline{\mathbf{S}}^t$ does not hold for Equation (19). However, another variational formula for capacitance extractions can still be constructed.

THEOREM 2 *Suppose that there are N conductors arbitrarily placed in an isotropic inhomogeneous medium environment. If the elastance matrix Equation (12) is asymmetrical, the mutual capacitance C_{ji} will be determined by the following variational formula*

$$C_{ji}^{-1} = \frac{\tilde{\mathbf{q}}^{jt} \cdot \overline{\mathbf{S}} \cdot \mathbf{q}^i}{Q_j^i \tilde{Q}_i^j} \tag{21}$$

where $\mathbf{q}^i$ and $\tilde{\mathbf{q}}^j$ are the charge vectors of all patches when only the ith or only the jth conductor is assigned nonzero potential. They satisfy

$$\overline{\mathbf{S}} \cdot \mathbf{q}^i = \mathbf{\Phi}^i \tag{22}$$

$$\overline{\tilde{\mathbf{S}}} \cdot \tilde{\mathbf{q}}^j = \tilde{\mathbf{\Phi}}^j \tag{23}$$

where

$$\overline{\tilde{\mathbf{S}}} = \overline{\mathbf{S}}^t. \tag{24}$$

and $\mathbf{\Phi}^i$ *and* $\tilde{\mathbf{\Phi}}^j$ *are the potential vectors of all patches.* Q^i_j *is the net charge on the* j*th conductor based on Equation (22) when the* i*th conductor has nonzero potential.* $\tilde{Q}^j_i$ *is the net charge on the* i*th conductor based on Equation (23) when the* j*th conductor has nonzero potential.*

Proof From Equations (22) and (23), assuming that $\mathbf{q}^i$ and $\tilde{\mathbf{q}}^j$ solve them exactly, we have from (21) that

$$\begin{aligned} C_{ji}V_j &= Q^j_i \\ C_{ji}\tilde{V}_j &= \tilde{Q}^j_i \end{aligned}$$

Using the same procedure for Equation (19) and the assumption of Equation (24), Equation (21) can be easily proved.

Then rewriting Equation (21) and taking the first order variation on both sides, we have

$$\delta C^{-1}_{ji} Q^i_j \tilde{Q}^j_i + C^{-1}_{ji}\delta Q^i_j \tilde{Q}^j_i + C^{-1}_{ji} Q^i_j \delta\tilde{Q}^j_i = \delta\tilde{\mathbf{q}}^{jt}\cdot\overline{\mathbf{S}}\cdot\mathbf{q}^i + \tilde{\mathbf{q}}^{jt}\cdot\overline{\mathbf{S}}\cdot\delta\mathbf{q}^i$$

The right hand side can be simplified by Equation (22) and (23) to

$$RHS = \delta\tilde{\mathbf{q}}^{jt}\cdot\mathbf{\Phi}^i + \tilde{\mathbf{\Phi}}^{jt}\cdot\delta\mathbf{q}^i = \delta\tilde{Q}^j_i V_i + \delta Q^i_j \tilde{V}_j$$

while the left hand side is

$$LHS = \delta C^{-1}_{ji} Q^i_j \tilde{Q}^j_i + \tilde{V}_j \delta Q^i_j + V_i \delta\tilde{Q}^j_i$$

then $\delta C^{-1}_{ji} = 0$.

Although it seems that THEOREM 1 is a special case of THEOREM 2 when $\tilde{\overline{\mathbf{S}}} = \overline{\mathbf{S}}$, THEOREM 1 agrees better with the original integral equation which is self-adjoint. THEOREM 2 is only a modified version of THEOREM 1 to deal with artifacts caused by numerical methods which destroy the symmetry of the system.

Hence the variational computation of mutual capacitances is always possible even when numerical artifacts are involved. However, the asymmetric form given by (21) requires the solving of the original and adjoint problem as given in (22) and (23). Therefore, its use is more costly than the symmetric form as given in (12).

3. FAST MULTIPOLE ALGORITHM

The charge distribution over conductors must be solved from generalized elastance matrix Equation (12) for capacitance extractions.

Fast multipole algorithm (FMA), combined with CG method, has been used as the solver [15, 21]. For multi-layer applications, a method considering the multi-reflection effects has been developed [19, 20]. FMA provides an efficient approach for obtaining the charge distributions on conductor surfaces. After the charge has been calculated, the variational formula (Equation (19)) or the direction capacitance formula (Equation (16)) can be used to compute the mutual and self-capacitances. Details about FMA will not be discussed in this paper.

4. NUMERICAL RESULTS

The generalized variational formula derived for capacitance extractions is tested using the FMA algorithm. The capacitance matrix of two unit perfect electric conducting spheres separated by 2.5 meters is computed. They are discretized into 6,400 triangles. Galerkin's method is applied using single precision, and the relative residual error limit of CG is 10^{-6}. The conventional method shown in Equation (16) and the new variational method shown in Equation (19) are tested. FMA is used to compute charge distributions. The multipole expansion truncation number p changes from 0 to 6. The capacitance matrix computed using $p = 8$ is set to be the reference (it will not be same as the analytic solution because of the geometrical modelling error due to the finite discretization of the geometry).

However, it is found that the variational method does not improve the accuracy if it is directly applied to the resultant charges using FMA computations (see the "variational form (a)" of Figure 1). The reason is that in low order FMA (p is small), due to the factorization of the Green's function, the equivalent elastance matrix $\overline{\mathbf{S}}$ has some error ($\delta\overline{\mathbf{S}}$). Then the variational formula will become

$$C_{ji}^{-1} = \frac{\mathbf{q}_j^t \cdot \overline{\mathbf{S}} \cdot \mathbf{q}_i}{Q_j^i Q_i^j} + \frac{\mathbf{q}_j^t \cdot \delta\overline{\mathbf{S}} \cdot \mathbf{q}_i}{Q_j^i Q_i^j} \tag{25}$$

The second term introduces errors which can overwhelm the accuracy improvement brought by the variational formula. To avoid this problem, the matrix-vector product, $\overline{\mathbf{S}} \cdot \mathbf{q}^i$, used in Equation (19) is evaluated more accurately by using higher order multipole expansion to reduce the error in the factorization of the Green's function. In this example, if the multipole number used for the charge computation is p, the matrix-vector product in the variational formula will use $p + 3$. Since the variational formula requires only one matrix-vector product after the iterative solver is used with many iterations to solve for the

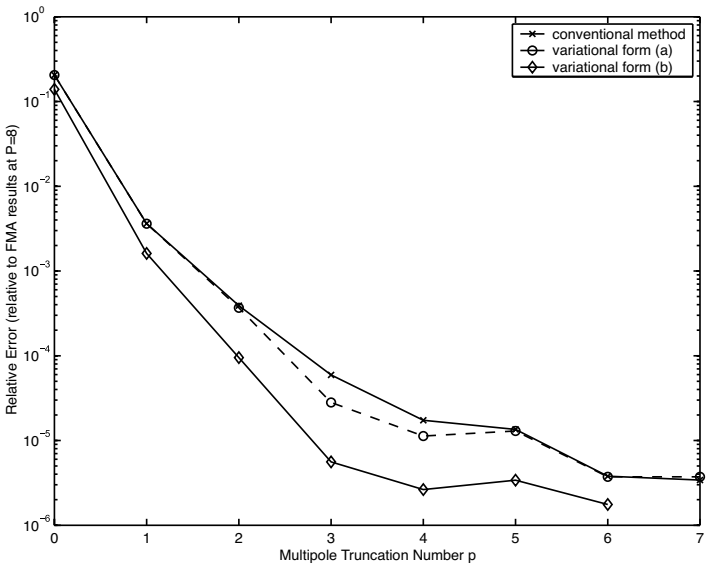

Figure 1. Accuracy enhancement by the variational formula.

charge, there will be no big cost increase. (This problem will not occur when Gaussian elimination is used to solve the matrix equation.) The improved result is plotted as "variational form (b)" in Figure 1. It can be seen that the variational formula brings significant accuracy improvement over the conventional data.

Another example is to compute the self and mutual capacitances of two unit spheres using Galerkin's method and CG. The charge distributions obtained from different stages of CG iteration are applied to the conventional direct capacitance formula (3) and the new variational formula (19). The capacitance error is relative to the capacitances computed from LU decomposition of (12) first for the charge $\mathbf{q}^i$ followed by the direct capacitance formula (3). The convergence error of the mutual capacitance and the self-capacitance are plotted in Figure 2. It can be seen that the variational method converges to 10^{-5} much faster than the direct method. It means that the variational method gives rise to faster convergence requiring less number of iterations.

To apply this method to the interconnect and packaging parasitic capacitance extraction, a two-signal-line example is studied. The geometry is shown in Figure 3. The method of moments is used to compute the capacitance matrix. The variational method is deployed to improve the accuracy of the results. To demonstrate the advantage

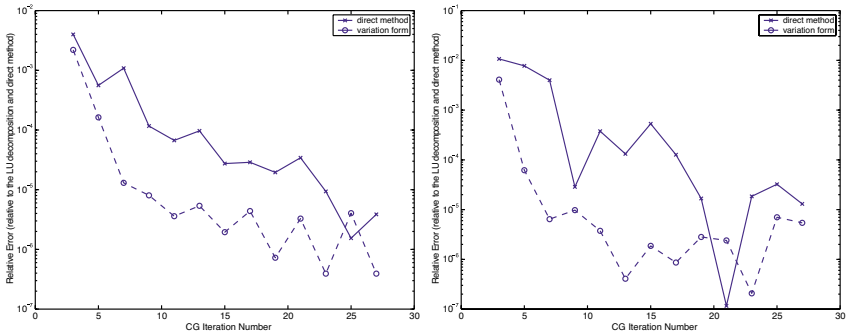

Figure 2. Accuracy enhancement by the variational formula. The left plot is for self-capacitance and the right plot is for mutual capacitance.

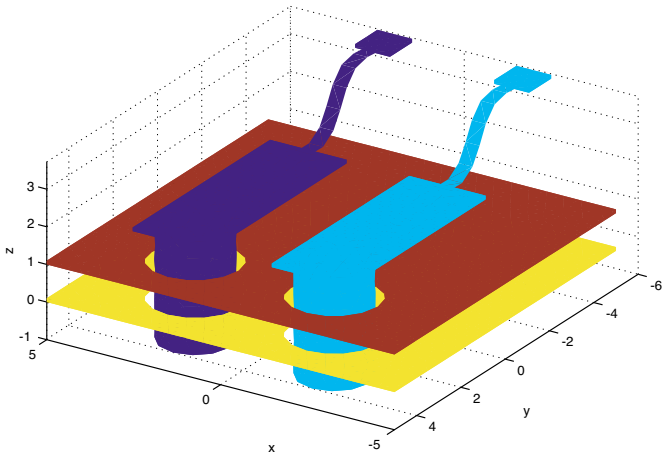

Figure 3. The geometry of the two signal lines. The two signal lines penetrate two isolated ground plates through vertical vias.

of the variational method over the direct method, the relative errors of the four components in the first row of the capacitance matrix are compared in Figure 4. The relative error is defined as the relative capacitance difference between two adjacent iterations:

$$E = \left| \frac{C_{ij}^{k-1} - C_{ij}^{k}}{C_{ij}^{k-1}} \right| \tag{26}$$

where C_{ij}^{k-1} is the extracted capacitance C_{ij} at the $(k-1)$-th iteration. From Figure 4, it is obvious that the variational method provides

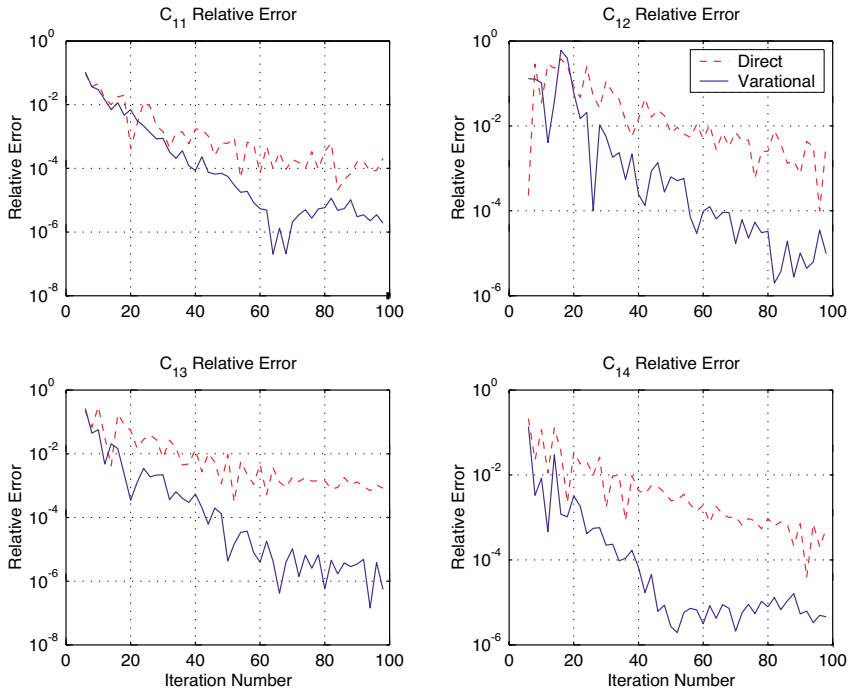

Figure 4. The relative error of four capacitance matrix elements using direct method and variational method for the two-signal-line benchmark shown in Figure 3.

a much faster convergence compared to the direct method for all capacitive couplings.

5. CONCLUSION

In this paper, a set of new variational formulas for capacitance extractions are derived. They are complete because they are valid not only for self-capacitances, but also for mutual capacitances. As for asymmetrical elastance matrix case resulting from the choice of numerical method, a new variational capacitance formula can still be derived. They gave higher accuracy compared to the conventional capacitance extraction methods.

The idea expounded in this paper can also be extended to other applications in large-scale computing where solution error persists due to the use of conjugate gradient method combined with fast algorithms. These methods often trade off accuracy with speed, but the use of

variational formulas to improve the accuracy of a desired parameter. In this paper, the parameter is the mutual or the self capacitance, but for other applications such as radar cross section computation, the use of variational formulas can accelerate the convergence of the radar cross section to the desired value.

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