Multipole Accelerated Capacitance Calculation for Structures with Multiple Dielectrics with high Permittivity Ratios

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Abstract— **This paper describes a new boundary integral formulation for the three-dimensional capacitance calculation of structures with multiple dielectrics. Unlike the existing equivalent-charge formulation, the new approach allows accurate numerical approximations when the permittivity ratios of the dielectrics are large. A multipole-accelerated algorithm based on this approach is described, and numerical results of its implementation are presented.**

I. Introduction

The self and coupling capacitances associated with integrated circuit interconnect and packaging are becoming increasingly important in determining final circuit performance and reliability. However, accurate estimation of these capacitances involves analyzing innately three-dimensional structures with dielectric materials surrounding conductors in a complicated fashion. Integrated circuits, for example, have multiple layers of polysilicon or metal conductors, separated by conformal or space-filling dielectrics. Also, packaging and off-chip interconnection problems often involve connectors passing through several plastic or ceramic dielectrics. The recent development of multipole-accelerated boundary-element methods for three-dimensional capacitance extraction has made accurate analysis of very complex structures in a uniform dielectric computationally inexpensive [1]. Moreover, the fast multipole method has been extended to problems where the conductors are surrounded by multiple dielectric regions of arbitrary shape, thus allowing the analysis of more realistic integrated circuit interconnect and packaging problems [6].

Traditionally, the extension to multiple dielectrics is based on the equivalent-charge approach. However, it has been observed by Nabors et al. [6] that this formulation can result in very poor numerical approximations of capacitances when the ratios of the involved permittivities are large.

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This article gives an explanation why any numerical scheme discretizing the equivalent-charge formulation will fail when the permittivity ratio is high enough. Furthermore, we present a modification which results in stable approximations of capacitances: the error of the modified method is independent of the permittivity ratio.

Section II briefly reviews the equivalent-charge formulation and describes the numerical problems in the case of high permittivity ratios. The following section proposes a modification of the existing technique which avoids the difficulties of the original formulation. The method's utility is demonstrated in Section V by applying our multipole-accelerated implementation of the algorithm to two examples.

II. Equivalent Charge Formulation

The equivalent charge approach [2], [3] to computing capacitances involves replacing the conductor surfaces S_c with a charge density σ_c and the dielectric interfaces S_d with a charge density σ_d. The potential produced by this combined density is then given by

$$\psi(x) = V_c\sigma_c(x) + V_d\sigma_d(x)\,, \qquad x \in \mathbf{R}^3\,. \tag{1}$$

Here V_c and V_d denote the potentials due to charges on S_c and S_d, respectively, which can be obtained by replacing S with the appropriate surface in the superposition integral

$$V\sigma(x) = \frac{1}{4\pi}\int_S \frac{1}{|x-y|}\,\sigma(y)\,dS(y)\,.$$

Note that we will use dimension-less notations throughout this article, i.e., we set the permittivity of the free-space to unity.

There are two types of boundary conditions which will determine the charge densities σ_c and σ_d. On the conductor surfaces the potential is specified, whereas on the interface of two dielectrics a condition on the potentials normal derivative is given. In particular, we have

$$\begin{aligned} \psi(x) &= 1\,, && x \in S_c \\ \varepsilon_a \tfrac{\partial \psi^a}{\partial n}(x) &= \varepsilon_b \tfrac{\partial \psi^b}{\partial n}(x)\,, && x \in S_d\,. \end{aligned} \tag{2}$$

Here n denotes the normal of the interface and ψ^a is the potential approached from the side of the interface with permittivity ε_a and ψ^b is the analogous potential for the

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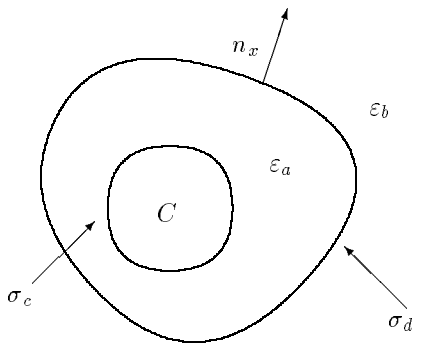

Fig. 1. Conductor C surrounded by dielectric materials with permittivities ε_a and ε_b

ε_b-side. The normal on the interface is chosen to point into the side of the lower permittivity.

It is well known that the electric field $V\sigma$ due to the surface charge σ is not continuous across this surface [7]. More precisely, we have jump relation for the normal component of the field

$$\frac{\partial}{\partial n_x}(V\sigma)(x) = \pm\frac{\sigma(x)}{2} + E\sigma(x), \qquad x \in S \tag{3}$$

where

$$E\sigma(x) = \frac{1}{4\pi}\int_S \frac{\partial}{\partial n_x}\frac{1}{|x-y|}\,\sigma(y)\,dS(y)\,. \tag{4}$$

The negative sign in the formula (3) is chosen for the field on the side of the surface in direction of the normal, the plus sign is for the opposite side. Subtracting the jump relation for both sides of the surface yields the important relation between the charge density and the jump of the electric field

$$\sigma = \frac{\partial \psi^b}{\partial n} - \frac{\partial \psi^a}{\partial n}\,. \tag{5}$$

From the formula above and the boundary conditions the following system of integral equation for the densities σ_c and σ_d can be derived

$$\begin{aligned} V_c\sigma_c(x) + V_d\sigma_d(x) &= f(x)\,, & x \in S_c \\ E_c\sigma_c(x) + \left(\tfrac{1}{2\lambda} + E_d\right)\sigma_d(x) &= 0\,, & x \in S_d\,. \end{aligned} \tag{6}$$

Here the operators E_c and E_d are defined by replacing S in (4) with the surfaces S_c and S_d, respectively, and the normal n_x with the normal of the dielectric interface. The parameter λ is given by

$$\lambda = \frac{\varepsilon_a - \varepsilon_b}{\varepsilon_a + \varepsilon_b}\,. \tag{7}$$

To determine the self capacitance of a conductor (for the case that only one conductor is present), the potential f on S_c is set to one volt. For mutual capacitances (in the case of multiple conductors) the right hand side f is set to one volt on one conductor and zero volts on the other conductors.

After the charge density σ_c has been determined, the capacitance of a conductor can be calculated by

$$C_\lambda = \varepsilon_a \int_{S_c} \sigma_c(y)\,dS(y)\,. \tag{8}$$

Typically, system (6) is discretized with piecewise constant collocation. Nabors et al. [6] observed in this context that the error of the numerically approximated solution grows rapidly as the ratio of the permittivities increases. In the same article they propose to employ the Galerkin method for the discretization of (6). Even though the Galerkin scheme improves the approximation, the method produces inaccurate results if the permittivity ratio becomes too high.

III. High Permittivity Ratios

For simplicity, consider one conductor raised to one volt which is embedded in a dielectric material, as depicted in Figure 1. To study large permittivities set $\varepsilon_b = 1$ and let $\varepsilon_a \to \infty$ which is equivalent to letting λ in (7) approach 1. Physically, the $\varepsilon_a \to \infty$ limit implies that the dielectric material is acting like a conductor. Hence all charges must be located on the dielectric interface and the conductor density must vanish.

Since there are no charges in the interior of the $\varepsilon_a = \infty$ dielectric, the potential, denoted by ψ_∞, is constant throughout the dielectric material and is therefore one volt on the dielectric interface. This boundary condition gives rise to the following integral equation for the charge density $\sigma_{d,\infty}$ on the interface

$$V_d\sigma_{d,\infty}(x) = 1\,, \qquad x \in S_d\,. \tag{9}$$

The latter problem is equivalent to calculating the capacitance of the structure where the dielectric material has been replaced by a conductor. Thus the original problem which was posed on S_c and S_d is reduced to a problem posed on S_d only. Moreover, the capacitance of this problem is given by

$$C_\infty = \int_{S_d} \sigma_{d,\infty}\,dS\,.$$

In view of the equivalent charge formulation, we see that $\sigma_c = 0$ and $\sigma_d = \sigma_{d,\infty}$ is the solution of (6) for $\lambda = 1$. The first equation is satisfied, because the potential $\psi_\infty \equiv 1$ in the interior of the dielectric medium. The second equation follows from the jump relation (3) and the fact that the electric field vanishes on the ε_a-side of the interface.

Now consider the solution σ_c, σ_d of the equivalent charge formulation (6) for large, but finite ε_a. From the previous discussion it is clear that σ_c is small compared to σ_d because σ_c converges to zero whereas σ_d converges to the non-zero charge $\sigma_{d,\infty}$.

When solving (6) numerically, the discretization error will be distributed evenly over both surfaces which results in large relative errors in the conductor surface charge. This has a severe effect for the approximation error of the capacitance. Because of the factor ε_a in (8), the discretization error of C_λ grows linearly with the permittivity for a fixed discretization. Note however, that the exact value of C_λ converges to C_∞. This can be seen by integrating the second equation in (6) over the interface S_d. By Gauss's law, we have $\int_{S_d} E_c \sigma_c = \int_{S_c} \sigma_c$ and $\int_{S_d} E_d \sigma_d = -1/2 \int_{S_d} \sigma_d$. Hence,

$$C_\lambda = \int_{S_c} \sigma_c = \varepsilon_a \Big(\frac{1}{2\lambda} - \frac{1}{2}\Big) \int_{S_d} \sigma_d \to C_\infty \,.$$

Thus we see that in the limit of $\varepsilon_a \to \infty$ the relative error of the capacitance grows without bounds.

IV. The Perturbation Approach

The major difficulty associated with high permittivity ratios is that the solution of the equivalent charge formulation (6) has different scales. The purpose of this section is to introduce a two step procedure which avoids different scaling of the densities on the conductor and dielectric surfaces. To obtain such a method we set up the potential as the combination of ψ_∞, the potential generated by $\varepsilon_a = \infty$, and a perturbation $\widetilde{\psi}$ accounting for the finite permittivity

$$\psi(x) = \psi_\infty(x) + \widetilde{\psi}(x) \,.$$

As was shown above, the potential ψ_∞ results only from the charge $\sigma_{d,\infty}$ on the interface, which is given by integral equation (9). This is a standard capacitance problem and can be solved numerically to high accuracy [1], [3].

The perturbation $\widetilde{\psi}$ is set up as a super-position of charges on the conductor surface and the dielectric interface, similar to the definition of the potential in (1)

$$\widetilde{\psi}(x) = V_c \widetilde{\sigma}_c(x) + V_d \widetilde{\sigma}_d(x) \,. \tag{10}$$

Substituting (10) into (2), we obtain a new set of boundary conditions for perturbation $\widetilde{\psi}$

$$\begin{aligned} \widetilde{\psi}(x) &= 0 \,, & x \in S_c \\ \varepsilon_a \tfrac{\partial \widetilde{\psi}^a}{\partial n}(x) &= \varepsilon_b \left(\tfrac{\partial \widetilde{\psi}^a}{\partial n}(x) - \sigma_{d,\infty}(x) \right) \,, & x \in S_d \,. \end{aligned} \tag{11}$$

The second equation holds because ψ_∞ is constant within the dielectric material and hence $\partial \psi^a_\infty / \partial n = 0$ and $\partial \psi^b_\infty / \partial n = -\sigma_{d,\infty}$ by the jump relation (5).

These boundary conditions yield, very much in the same way as for (6), the following system of integral equations for the perturbations $\widetilde{\sigma}_c$ and $\widetilde{\sigma}_d$

$$\begin{aligned} V_c \widetilde{\sigma}_c(x) + V_d \widetilde{\sigma}_d(x) &= 0 \,, & x \in S_c \\ E_c \widetilde{\sigma}_c(x) + (\tfrac{1}{2\lambda} + E_d) \widetilde{\sigma}_d(x) &= \tfrac{\lambda - 1}{\lambda} \sigma_{\infty,d}(x) \,, & x \in S_d \,. \end{aligned} \tag{12}$$

Since the potential ψ_∞ is generated only by charges on the dielectric interface, we see that $\widetilde{\sigma}_c = \sigma_c$. Hence the capacitance (8) is given by

$$C = \varepsilon_a \int_{S_c} \frac{1}{|x-y|} \widetilde{\sigma}_c(y) \, dS(y) \,. \tag{13}$$

The system above has the same operator on the left hand side as the original system (6), only the right hand side has changed. This is the key observation. The right hand side is $\mathcal{O}(1/\varepsilon_a)$ as $\varepsilon_a \to \infty$. Hence, by linearity, we see that $\widetilde{\sigma}_c$ and $\widetilde{\sigma}_d$ are both $\mathcal{O}(1/\varepsilon_a)$ and therefore there is no different scaling in the solution of equation (12).

By the same argument the error due to discretizing (12) scales like $\mathcal{O}(1/\varepsilon_a)$. Hence the error of the capacitance in (13) can be bounded independently of the permittivity ε_a.

The perturbation approach for calculating capacitances of structures involving dielectrics with high permittivies can be summarized as follows.

1. Solve problem (9) on the conductor surface for ρ_d.
2. Solve the perturbation equation (12).
3. Calculate the capacitance via formula (13).

V. Results

To demonstrate the accuracy of the capacitance extraction algorithm described in this article, the capacitances with two test problems were computed. The calculations are based on the package `FASTCAP` [1] with some modifications to facilitate solving the new integral formulation discussed in Section IV. The numerical method used here is piecewise constant collocation with sparsification of the resulting system matrix by the Fast Multipole Method [5], [4].

In the first example we approximate the capacitance of the unit radius spherical conductor which is covered by a unit thick coating.

The analytic values of the capacitance are compared with the numerical results generated by the equivalent charge and by the modified formulation. For both calculations, we used the same discretization into 1536 panels. Figure 2 shows the relative errors for a wide range of permittivity ratios. As it can be seen from this plot, the equivalent charge approach gives very poor approximations for high permittivity ratios, whereas the the error of our modified method remains bounded, even when $\varepsilon_a \to \infty$.

To demonstrate that the modified formulation is also useful for more complex geometries, the capacitances associated with the bus-crossing structure of Figure 3 are calculated.

Table I compares the calculated coupling capacitances derived from raising conductor three to one volt for the two approaches described in this article. Both formulations agree (up to marginal differences) on the self capacitance and the coupling capacitance to conductor four.

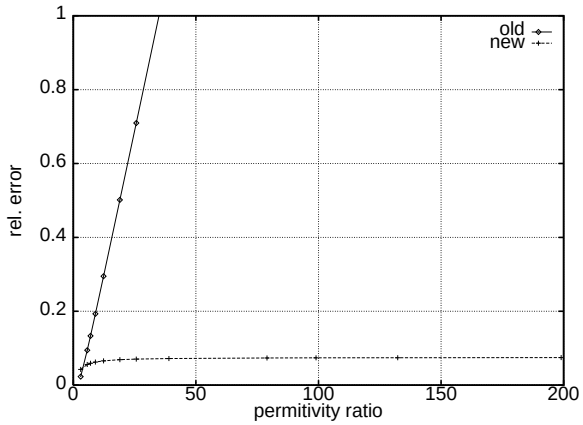

Fig. 2. Relative errors of the capacitance as calculated by the equivalent charge formulation (Method 1) and the modified formulation (Method 2). Coated sphere example. The exact value of the capacitance varies between 18 and 25.

However, there is a significant difference in the two approaches for the coupling between conductor three and the conductors surrounded by the dielectric. It appears that the results given by the equivalent charge formulation are too high. In fact, the experiments showed that for increasing permittivity ratios these capacitances diverge for the equivalent charge approach, but approached a fixed limit for our modified formulation.

Cap.	ε_a	2	4	6	8	10
C_{31}	old	-12.3	-15.3	-17.3	-19.0	-20.5
	new	-11.8	-13.9	-14.8	-15.3	-15.7
C_{32}	old	-12.3	-15.3	-17.3	-19.0	-20.4
	new	-11.8	-13.9	-14.8	-15.3	-15.7
C_{33}	old	39.1	43.0	44.8	45.8	46.5
	new	39.5	43.8	45.8	46.9	47.6
C_{34}	old	-8.1	-7.8	-7.7	-7.7	-7.6
	new	-8.1	-7.8	-7.7	-7.6	-7.6

TABLE I

Comparison of the calculated coupling capacitances for various permittivities from conductor three. Bus crossing example in Figure 3, 'old' refers to the equivalent charge formulation, 'new' to the perturbation method.

VI. Conclusion

The capacitance calculation for structures with multiple dielectrics by the equivalent charge formulation can be erroneous when the ratio of the permittivities is high. The modified formulation described in this article does not suffer from an accuracy loss in this case. Furthermore, calculations via the new approach can be multipole-accelerated and are therefore efficient enough to allow capacitance extractions of complex three-dimensional, multiple-dielectric geometries.

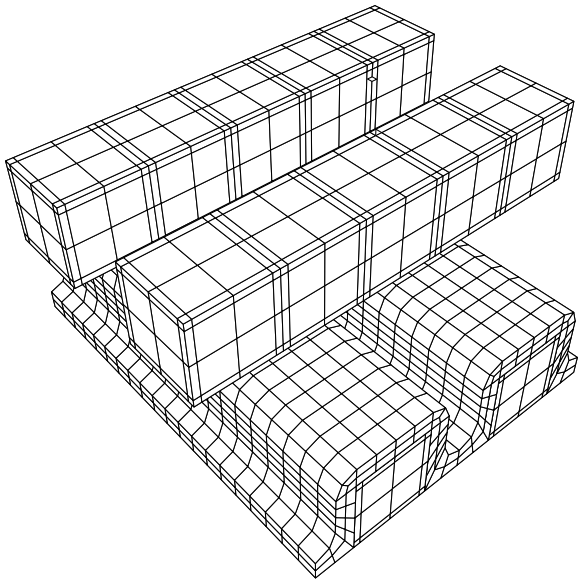

Fig. 3. The bus crossing example. The two bottom conductors are numbered 1 and 2, the two top conductors 3 and 4.

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