Multipole-Accelerated 3-D Capacitance Extraction Algorithms for Structures with Conformal Dielectrics

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Abstract

The new three-dimensional capacitance calculation program FASTCAP2 is described. Like the earlier program, FASTCAP, FASTCAP2 is based on a multipole-accelerated algorithm that is efficient enough to allow three-dimensional capacitance calculations to be part of an iterative design process. FASTCAP2 differs from FASTCAP in that it is able to analyze problems with multiple dielectrics, thus extending the applicability of the multipole-accelerated approach to a wider class of integrated circuit interconnect and packaging problems.

1 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 [5]. This paper extends the original method 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.

The following section describes the equivalent-charge approach to analyzing structures with dielectric interfaces. Section 3 then shows how this formulation can be used as a framework for a multipole-accelerated iterative solution method. The method's utility is demonstrated in Section 4 by applying our implementation of the algorithm, FASTCAP2, to several examples.

2 Equivalent-Charge Formulation

To determine all the self and coupling capacitances of a structure with m conductors, the conductor surface charges must be computed m times, with m different sets of conductor potentials. In particular, if conductor i is raised to unit potential and the rest are grounded, then the total charge on conductor i is numerically equal to conductor i's self capacitance. Furthermore, any other conductor's total charge is numerically equal to the negative of its coupling capacitance to conductor i.

Given the conductor potentials, the conductor surface charges can be computed by replacing the conductor-dielectric and dielectric-dielectric interfaces with a surface charge layer of density $\sigma(x)$ and changing all the dielectric regions to free space. Then in this equivalent free-space problem, $\sigma(x)$ is determined by insisting that it produce a potential which matches conductor potentials at conductor-dielectric interfaces, and satisfies normal electric-field conditions at the dielectric-dielectric interfaces [2, 6].

To numerically compute σ, the conductor surfaces

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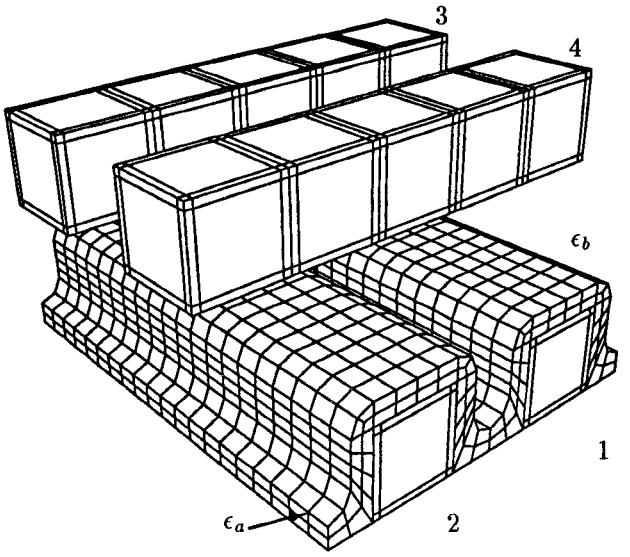

Figure 1: The panels used to discretize a 2×2 dielectric-coated bus-crossing problem. The lower conductors' surfaces are discretized in the same way as the two upper conductors' surfaces.

and dielectric interfaces are discretized into $n = n_p + n_d$ small panels or tiles, with n_p panels on conductor surfaces and n_d panels on dielectric interfaces as in Figure 1. It is then assumed that on each panel i, a charge, q_i, is uniformly distributed. For each conductor surface panel, an equation is written which relates the potential at the center of that i-th panel, denoted p_i, to the sum of the contributions to that potential from the n charge distributions on all n panels. For example, the contribution of the charge on panel j to the potential at the center of panel i is given by the superposition integral

$$\frac{q_j}{a_j}\int_{panel\ j}\frac{1}{4\pi\epsilon_0\|x_i - x'\|}\,da', \qquad (1)$$

where x_i is the center of panel i, a_j is the area of panel j, ϵ_0 is the permittivity of free space, and the constant charge density q_j/a_j has been factored out of the integral. The total potential at x_i, is the sum of the contributions from all n panels,

$$p_i(x_i) = P_{i1}q_1 + P_{i2}q_2 + \cdots + P_{ij}q_j + \cdots + P_{in}q_n, \quad (2)$$

where

$$P_{ij} \triangleq \frac{1}{a_j}\int_{panel\ j}\frac{1}{4\pi\epsilon_0\|x_i - x'\|}\,da'. \qquad (3)$$

Similarly, for each dielectric interface panel, an equation is written that relates the normal displacement-field difference at the center of that i-th dielectric interface panel to the sum of the contributions to that displacement field due to the n charge distributions on all n panels. In particular, if panel i lies on the interface between dielectrics with permittivities ϵ_a and ϵ_b, then the Gauss's Law condition

$$\epsilon_a\frac{\partial p_i(x_i)}{\partial n_i} - \epsilon_b\frac{\partial p_i(x_i)}{\partial n_i} = 0 \qquad (4)$$

must hold. Here n_i is a normal to panel i. Substituting the expression (2) breaks (4) into a superposition over all the panels,

$$D_{i1}q_1 + D_{i2}q_2 + \cdots + D_{ij}q_j + \cdots + D_{in}q_n = 0, \quad (5)$$

where

$$D_{ij} \triangleq (\epsilon_a - \epsilon_b)\frac{\partial}{\partial n_i}\frac{1}{a_j}\int_{panel\ j}\frac{1}{4\pi\epsilon_0\|x_i - x'\|}\,da'. \quad (6)$$

Careful evaluation of the derivative in (6) leads to the important special case [3]

$$D_{ii} \triangleq \frac{(\epsilon_a + \epsilon_b)}{2\epsilon_0}. \qquad (7)$$

Collecting all n equations of the form (2) and (5) leads to the dense linear system

$$\begin{bmatrix} P_{11} & \cdots & P_{1n} \\ \vdots & & \vdots \\ P_{n_p1} & \cdots & P_{n_pn} \\ D_{n_p+1,\,1} & \cdots & D_{n_p+1,\,n} \\ \vdots & & \vdots \\ D_{n1} & \cdots & D_{nn} \end{bmatrix}\begin{bmatrix} q_1 \\ \vdots \\ q_{n_p} \\ q_{n_p+1} \\ \vdots \\ q_n \end{bmatrix} = \begin{bmatrix} p_1 \\ \vdots \\ p_{n_p} \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad (8)$$

or

$$\begin{bmatrix} P \\ D \end{bmatrix}[\ q\ ] = \begin{bmatrix} p \\ 0 \end{bmatrix}, \qquad (9)$$

where $P \in \mathbf{R}^{n_p \times n}$ is the matrix of potential coefficients, $D \in \mathbf{R}^{n_d \times n}$ is the matrix representing the dielectric interface boundary conditions, $q \in \mathbf{R}^n$ is the vector of panel charges, and $p \in \mathbf{R}^{n_p}$ is the vector of conductor-panel center-point potentials. Using

$$A \triangleq \begin{bmatrix} P \\ D \end{bmatrix}, \qquad b \triangleq \begin{bmatrix} p \\ 0 \end{bmatrix}, \qquad (10)$$

gives

$$Aq = b \qquad (11)$$

as the linear system to solve to for the conductor charge densities. In the standard approach the $n \times n$ linear system (11) is solved using a Gaussian elimination algorithm at a cost of order n^3 operations [8, 6]. Our algorithm uses the multipole-accelerated iterative method of the next section which requires only order mn operations.

3 The Multipole Approach

The dense linear system of (11) can be solved to compute panel charges from a given set of panel potentials, and the capacitances can be derived by summing the panel charges. If Gaussian elimination is used to solve (11), the number of operations is order n^3. Clearly, this approach becomes computationally intractable if the number of panels exceeds several hundred. Instead, consider solving the linear system (11) using a conjugate-residual style iterative method like GMRES [9]. Such methods have the form given below:

Algorithm 1: GMRES algorithm for solving (11)
Make an initial guess to the solution, q^0.
Set $k = 0$.
do {
  Compute the residual, $r^k = b - Aq^k$.
  if $||r|| < tol$, return q^k as the solution.
  else {
    Choose α's and β in
      $q^{k+1} = \sum_{j=0}^{k} \alpha_j q^j + \beta r^k$
    to minimize $||r^{k+1}||$.
    Set $k = k + 1$.
  }
}

Here $||\cdot||$ is the Euclidean norm. The dominant costs of this strategy are calculating the n^2 entries of A using (3) and (6) before the iterations begin, and then performing n^2 operations to compute the matrix-vector product Aq^k on each iteration. It is possible to avoid forming most of A and to substantially reduce the cost of computing Aq^k if an approximation to Aq^k can be tolerated [7].

The approximation used here is the multipole algorithm, an efficient way of calculating the potential due to a charge distribution in free space that reduces the cost of forming Aq^k to order n operations [1]. This does not necessarily imply that each iteration of the GMRES algorithm can be computed with order n operations. If the number of GMRES iterations required to achieve convergence approaches n, then the minimization in each GMRES iteration requires order n^2 operations. This problem is avoided through the use of a preconditioner which reduces the number of GMRES iterations required to achieve convergence to well below n for large problems [4].

The product Aq^k is, using (9),

$$Aq^k = \begin{bmatrix} Pq^k \\ Dq^k \end{bmatrix}. \qquad (12)$$

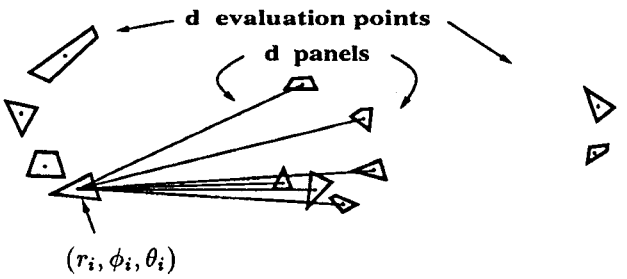

Figure 2: The direct evaluation of the potential due to d panel charges at d points.

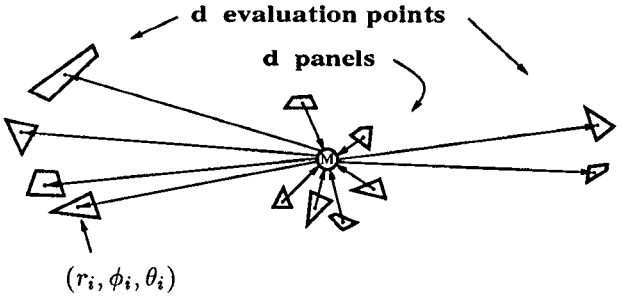

Figure 3: The evaluation of a the potential due to d panel charges at d points using a multipole expansion.

Forming the product Pq^k is equivalent to calculating the potential at all the conductor panel center points, making it possible to approximate it directly with the fast multipole algorithm. Although Dq^k has the dimensions of electric displacement, it can be expressed in terms of potential evaluations, leading to fast evaluation with the multipole algorithm.

3.1 Potential Evaluations

The key approximation employed in the multipole algorithm is the evaluation of potentials using multipole expansions. Consider evaluating the potential at d panel centers due to charges on another d panels as in Figure 2. In a direct evaluation, a single panel's center-point potential is calculated using an explicit equation like (2). In the Figure 2 case, d $P_{ij}q_j$ products are computed and added at a cost of d operations. Repeating the process for all d evaluation points requires d^2 operations.

When the charge panels are well-separated from the evaluation points the potentials can be approximated at much lower cost using a multipole expansion. A multipole expansion is a truncated series expansion of

the form

$$p_i(r_i, \phi_i, \theta_i) \approx \sum_{j=0}^{l} \sum_{k=-j}^{j} \frac{M_j^k}{r_i^{j+1}} Y_j^k(\phi_i, \theta_i). \qquad (13)$$

where (r_i, ϕ_i, θ_i) are the spherical coordinates of panel i's center point (the evaluation point) measured relative to the origin of the multipole expansion, $Y_k^j(\phi_i, \theta_i)$ are the surface spherical harmonics, l is the expansion order, and M_k^j are the multipole coefficients which are determined from the well-separated panel charges using

$$M_j^k \triangleq \sum_{i=1}^{d} \frac{1}{a_i} \int_{panel\ i} (\rho')^j Y_j^{-k}(\alpha', \beta') da'. \qquad (14)$$

The use of the expansion is illustrated in Figure 3. A single multipole expansion for the potential due to the d panel charges is evaluated at the d evaluation points. Since the expansion is used many times, the cost of computing it may be neglected. Thus the multipole evaluation of the same d potentials requires only d operations.

The reduction in complexity resulting from the aggregation of distant panels into multipole expansions which can be used to evaluate potentials at many panel centers is the source of the multipole algorithm's efficiency. Maintaining this efficiency for general distributions of panels while controlling error leads to the hierarchical multipole algorithm used in FASTCAP2. A detailed description of the complete multipole algorithm is given in [1] and its use in the context of capacitance extraction is described in [5, 4].

3.2 Electric Field Evaluations

The evaluation of Dq^k amounts to calculating the left-hand side of n_d equations of the form (5) or, equivalently, (4). The left-hand side of (4) can be approximated by replacing the derivatives by divided differences constructed near panel i as illustrated in Figure 4, yielding

$$\epsilon_a \frac{\partial p_i}{\partial n_i} - \epsilon_b \frac{\partial p_i}{\partial n_i} \approx \epsilon_a \frac{(p_i - p_a)}{h} - \epsilon_b \frac{(p_b - p_i)}{h}. \qquad (15)$$

Thus the n multiply-adds required to find one inner product in Dq^k are replaced by three multipole algorithm potential evaluations followed by the divided difference calculation (15). In this way the bulk of the displacement field calculation is performed using the efficient multipole algorithm to compute the potentials $p_i(x_i)$, $p_a(x_a)$ and $p_b(x_b)$.

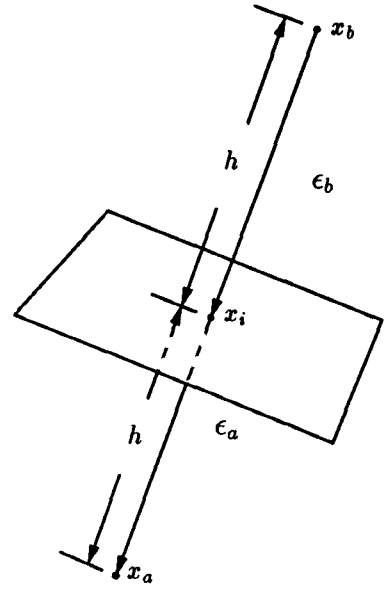

Figure 4: The electric fields on both sides of the dielectric panel are approximated with divided differences.

4 Results

To demonstrate the efficiency and accuracy of the multipole-accelerated capacitance extraction algorithm for problems with multiple dielectrics, the capacitances associated with the easily parameterized bus-crossing structure of Figure 1 are calculated. The Figure 1 problem is called the 2×2 bus-crossing problem and is representative of the 1×1 through 5×5 bus-crossings examined here. In all these problems the lower bus is covered with a layer of conformal dielectric with permittivity $\epsilon_a = 7.5\epsilon_0$ while the surrounding material has permittivity $\epsilon_b = 3.9\epsilon_0$. All the conducting bars have 1μm $\times 1\mu$m cross-sections, and all overhang and inter-conductor spacings are 1μm. The conformal dielectric is nominally 0.25μm thick.

The accuracy attained by our program, FASTCAP2, is investigated using the Figure 1 problem. The smallest coupling and self capacitances in the problem are calculated using FASTCAP2 and by Gaussian elimination applied directly to (11), the standard direct method. The entries in Table 1 represent the capacitances associated with the top, rear conductor in Figure 1. By default FASTCAP2 is configured to produce capacitances within 1% of those calculated using direct factorization, as is clearly the case here. Thus any error in the FASTCAP2 capacitances is dominated by discretization error rather than multipole approximation effects.

	C_{31}	C_{32}	C_{33}	C_{34}
Direct	−0.2112	−0.2112	0.9854	−0.3200
FASTCAP2	−0.2113	−0.2112	0.9886	−0.3212

Table 1: Comparison of capacitances (in fF) for the Figure 1 problem.

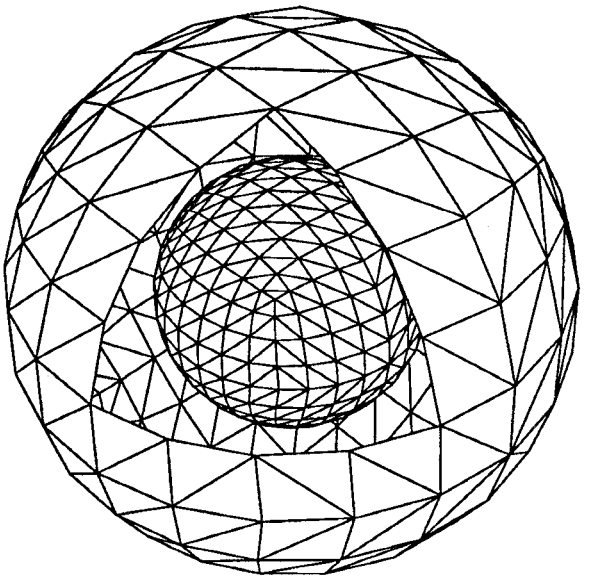

Figure 5: The discretization used to compute the capacitance of a dielectric-coated sphere in free space. Some of the outer dielectric-boundary panels have been removed to show the inner conductor surface panels.

Using the dielectric-coated sphere of Figure 5, FASTCAP2's accuracy is further demonstrated by comparing its result to an analytic value. The inner conducting sphere of radius 1m is coated by a 1m thick dielectric layer with relative permittivity 2. The surrounding region is free space. By Gauss's Law, such a structure has capacitance 148.35pF. The value calculated using FASTCAP2 applied to the discretization of Figure 5 is 148.5pF, well within 1% of the analytic value.

The program's execution speed for the four bus-crossing problems is compared to the speed of the standard direct method in Table 2. The values in parenthesis indicate extrapolated execution times corresponding to problems that could not be solved using the standard method due to excessive memory and time requirements. FASTCAP2's lower complexity leads to much lower execution times for even moderate sized problems like the 2×2 bus crossing. In particular, in the time required to compute the capacitance of the 4×4 bus crossing problem using standard direct methods, FASTCAP2 can perform seventy such calculations.

Problem	1×1	2×2	3×3	4×4
Panels	664	1984	3976	6640
Direct	1.4	41	(320)	(1400)
FASTCAP2	0.44	2.4	8.6	20

Table 2: Comparison of execution times in I.B.M. RS600/540 CPU minutes. Values in parenthesis are extrapolated.

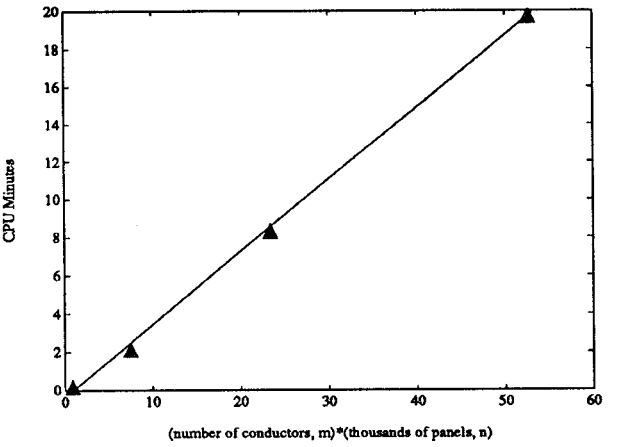

Figure 6: Demonstration of the order mn complexity of FASTCAP2 using the four bus crossing execution times. Times in CPU minutes on an I.B.M. RS6000/540.

Finally, FASTCAP2's execution time is shown to grow roughly linearly with mn, where m is the number of conductors and n is the number of panels. Figure 6 plots the FASTCAP2 execution times in Table 2 verses mn for the bus-crossing problems. As is illustrated, the execution time data points closely follow the best-fit straight line, indicating order mn complexity.

As a final example of the kind of analysis made possible by FASTCAP2, consider the connector in Figure 7. The U-shaped polyester body has a relative permittivity of 3.5; the pins have 0.65mm×0.65mm cross-sections and are spaced 3.25mm center to center. Connectors of this type must be analyzed carefully when used for high-speed bus connections [10]. Using a 9524-panel discretization, FASTCAP2 com-

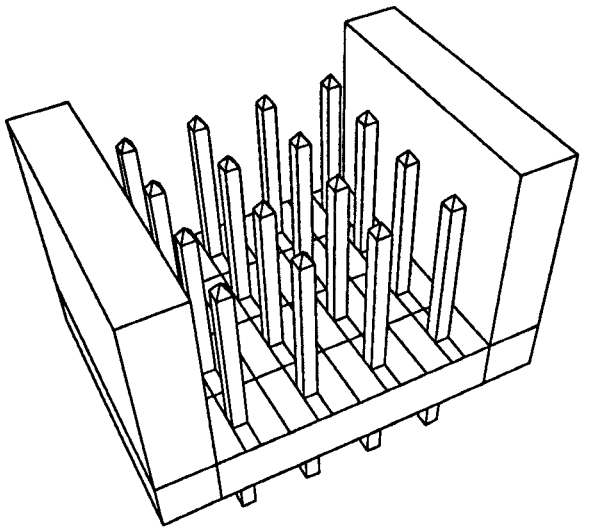

Figure 7: The backplane connector example.

putes all the self and coupling capacitances for the pins in thirty CPU minutes on an IBM RS6000/540. An identical analysis using standard Gaussian elimination algorithms requires roughly eight CPU days on the same machine. The four pins in the the center have the highest self capacitances: 0.547pF. The lowest self capacitance is 0.481pF and is attained by the four corner pins. The strongest coupling capacitances, slightly more than 0.2pF, occur between pin pairs next to the sides of the connector body. By grounding four pins on a diagonal and the four pins on the remaining parallel two-pin diagonals, the maximum signal pin coupling capacitance is reduced to around 0.065pF.

5 Conclusion

The multipole-accelerated capacitance extraction algorithm has been extended to problems with arbitrarily shaped, multiple-dielectric regions. The extended algorithm as implemented in FASTCAP2 has the same 1% accuracy and reduced time and memory requirements of the original algorithm. In particular, FASTCAP2 is fast enough to allow capacitance extraction of complex three-dimensional, multiple-dielectric geometries to be part of an iterative design process.

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