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Efficient Galerkin Techniques for Multipole-Accelerated Capacitance Extraction of 3-D Structures with Multiple Dielectrics

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Abstract

This paper describes an efficent implementation of a Galerkin based multipole-accelerated boundary-element method for 3-D capacitance extraction of conductors in an arbitrary piecewise-constant dielectric medium. Results are presented to demonstrate that the Galerkin method is substantially more accurate than the commonly used collocation scheme for problems with dielectric interfaces. In addition, it is shown experimentally that for a given discretization, a careful implementation of the Galerkin method in a multipole-accelerated program is only slightly more computationally expensive than the collocation method.

1 Introduction

The self and coupling capacitances associated with integrated-circuit interconnect and packaging are becoming increasingly important in determining final circuit performance and signal integrity. This has increased interest in computationally efficient procedures for determining capacitances of general three-dimensional structures. One recently developed approach to capacitance computation, the multipole-accelerated boundary-element method, can accurately analyze complex structures extremely efficiently[1, 2], provided it can be assumed that the dielectric is homogenous. For realistic problems, however, the dielectric inhomogeneity can not be ignored. For example, integrated circuit interconnect consists of multiple layers of polysilicon or metal conductors, separated by conformal or space-filling insulators with very different dielectric constants. In packaging and off-chip interconnect, conductors typically pass through plastic or ceramic holders with large relative dielectric constants.

In this paper we describe how to extend the multipole-accelerated boundary-element method to the case where conductors are embedded in an arbitrary piecewise-constant dielectric medium. In addition, we show that to achieve accurate results with reasonable discretizations, it is necessary to use Galerkin rather than collocation schemes. We start, in the next section, by reviewing the collocation-based multipole-accelerated boundary-element method for three-dimensional capacitance calculations. In Section 3, we derive the formulas needed to efficiently implement a Galerkin-based multipole-accelerated algorithm. In Section 4, results are presented to demonstrate that the Galerkin method is substantially more accurate than the collocation method for problems with dielectric interfaces, and it is shown that for a given discretization, a careful implementation of the Galerkin method in a multipole-accelerated program is only slightly more computationally expensive than the collocation method.

2 Standard Collocation Formulation

In this section we describe the multipole-accelerated algorithms currently used in the FASTCAP program to calculate the capacitance of conductors in multiple dielectric regions [3].

2.1 Equation 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 set to zero, 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 using an equivalent charge formulation. In this formulation, surface charge layers are placed at the conductor-dielectric and dielectric-dielectric interfaces, with densities $\sigma_c(x)$ and $\sigma_d(x)$ respectively, and the problem domain is replaced with free space. These surface charges therefore produce a potential given by

$$\psi(x) = \int_{S_c} \sigma_c(x') \frac{1}{4\pi\epsilon_0 \|x - x'\|} dS' + \int_{S_d} \sigma_d(x') \frac{1}{4\pi\epsilon_0 \|x - x'\|} dS', \tag{1}$$

where S_c and S_d are the conductor-dielectric and dielectric-dielectric interface surfaces. The densities $\sigma_c(x)$ and $\sigma_d(x)$ are determined in this equivalent free space problem by insisting that $\psi(x)$ match the conductor potentials for the original problem at conductor-dielectric interfaces, and that the normal derivative of the potential satisfy

$$\epsilon_a \frac{\partial \psi_+(x)}{\partial n_a} - \epsilon_b \frac{\partial \psi_-(x)}{\partial n_a} = 0, \quad x \in \epsilon_a, \epsilon_b \text{ interface}, \tag{2}$$

at any point x on a dielectric-dielectric interface. Here n_a is the normal to the dielectric interface at x that points into dielectric a, ϵ_a and ϵ_b are the permittivities of the corresponding linear, isotropic dielectric regions, $\psi_+(x)$ is the potential at x approached from the ϵ_a side of the interface, and $\psi_-(x)$ is the analogous potential for the b side [4, 5].

2.2 Collocation Discretization

To numerically compute σ_c and σ_d, the conductor surfaces and dielectric interfaces are discretized into $n = n_c + n_d$ small panels or tiles, with n_c panels on conductor surfaces and n_d panels on dielectric interfaces. 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

$$\frac{q_j}{a_j} \int_{panel\ j} \frac{1}{4\pi\epsilon_0 \|x_i - x'\|} da', \tag{3}$$

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,

$$p(x_i) = P_{i1}q_1 + P_{i2}q_2 + \cdots + P_{ij}q_j + \cdots + P_{in}q_n, \tag{4}$$

where

$$P_{ij} \triangleq \frac{1}{a_j} \int_{panel\ j} \frac{1}{4\pi\epsilon_0 \|x_i - x'\|}\, da'. \tag{5}$$

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 from (2),

$$\epsilon_a \frac{\partial p(x_{i_a})}{\partial n_i} - \epsilon_b \frac{\partial p(x_{i_b})}{\partial n_i} = 0. \tag{6}$$

Here, n_i is a normal to panel i, and x_{i_a} and x_{i_b} are x_i approached from the ϵ_a and ϵ_b sides of the interface, respectively. Substituting for p from (4) breaks (6) into a sum over all the panels,

$$D_{i1}q_1 + D_{i2}q_2 + \cdots + D_{ij}q_j + \cdots + D_{in}q_n = 0, \tag{7}$$

where

$$D_{ij} \triangleq (\epsilon_a - \epsilon_b) \frac{\partial}{\partial n_i} \frac{1}{a_j} \int_{panel\ j} \frac{1}{4\pi\epsilon_0 \|x_i - x'\|}\, da', \qquad i \neq j, \tag{8}$$

since if evaluation point j is not on panel i the limits $x_{i_a} \longrightarrow x_i$ and $x_{i_b} \longrightarrow x_i$ just replace the intermediate variables with x_i.

Careful evaluation of the limits when $i = j$ leads to the important special case [6]

$$D_{ii} \triangleq \frac{(\epsilon_a + \epsilon_b)}{2a_i\epsilon_0}. \tag{9}$$

Collecting all n equations of the form (4) and (7) leads to the dense linear system

$$\begin{bmatrix} P_{11} & \cdots & P_{1n} \\ \vdots & & \vdots \\ P_{n_c1} & \cdots & P_{n_cn} \\ D_{n_c+1,\,1} & \cdots & D_{n_c+1,\,n} \\ \vdots & & \vdots \\ D_{n1} & \cdots & D_{nn} \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_{n_c} \\ q_{n_c+1} \\ \vdots \\ q_n \end{bmatrix} = \begin{bmatrix} p_1 \\ \vdots \\ p_{n_c} \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{10}$$

A more convenient form of (10) is derived by rescaling the rows by $\frac{1}{\epsilon_a - \epsilon_b}$, which yields

$$\begin{bmatrix} P_{11} & \cdots & P_{1n} \\ \vdots & & \vdots \\ P_{n_c1} & \cdots & P_{n_cn} \\ E_{n_c+1,\,1} & \cdots & E_{n_c+1,\,n} \\ \vdots & & \vdots \\ E_{n1} & \cdots & E_{nn} \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_{n_c} \\ q_{n_c+1} \\ \vdots \\ q_n \end{bmatrix} = \begin{bmatrix} p_1 \\ \vdots \\ p_{n_c} \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \tag{11}$$

where E_{ij}, $i \neq j$, is just the normal electric field at x_i due to a unit charge on panel j, and is given by

$$E_{ij} \triangleq \frac{\partial}{\partial n_i} \frac{1}{a_j} \int_{panel\ j} \frac{1}{4\pi\epsilon_0 \|x_i - x'\|}\, da', \qquad i \neq j. \tag{12}$$

Note that just like D_{ii}, E_{ii} is a special case, and is given by

$$E_{ii} \triangleq \frac{(\epsilon_a + \epsilon_b)}{2a_i\epsilon_0(\epsilon_a - \epsilon_b)}. \tag{13}$$

We will write this compactly as

$$\begin{bmatrix} P \\ E \end{bmatrix} [\ q\ ] = \begin{bmatrix} p \\ 0 \end{bmatrix}, \tag{14}$$

where $P \in \mathbf{R}^{n_c \times n}$ is the matrix of potential coefficients, $E \in \mathbf{R}^{n_d \times n}$ is the matrix of electric field coefficients, $q \in \mathbf{R}^n$ is the vector of panel charges, and $p \in \mathbf{R}^{n_c}$ is the vector of conductor-panel center-point potentials. Using

$$A \triangleq \begin{bmatrix} P \\ E \end{bmatrix}, \qquad b \triangleq \begin{bmatrix} p \\ 0 \end{bmatrix}, \tag{15}$$

gives

$$Aq = b \tag{16}$$

as the linear system to solve to for the conductor charge densities.

2.3 Matrix Solution

The standard approach to solving the $n \times n$ linear system (16) is to use Gaussian elimination, at a cost of order n^3 operations [7, 5]. For this reason, the equivalent charge formulation approach to capacitance calculation is frequently considered computationally intractable if the number of panels exceeds several hundred. To improve the situation, consider solving (16) using a conjugate-residual style iterative method like GMRES [8]. Such methods have the general form below:

Algorithm 1: GMRES algorithm for solving (16)
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 $k = k + 1$.
  }
}

If GMRES is used to solve (16), and assuming few iterations are required to achieve GMRES convergence, the dominant costs of the approach are calculating the n^2 entries of A from (5) and (12), and performing n^2 operations to compute Aq^k on each GMRES iteration. In the next section, we will describe an approach to computing Aq^k which eliminates the need to form most of A, and produces an approximation to Aq^k in order n operations [9].

It should be noted that when applied to solving (16), the standard GMRES algorithm frequently requires a large number of iterations to achieve convergence. If the number of GMRES iterations approaches n, then the minimization in each GMRES iteration will require order n^2 operations, and the whole algorithm becomes order n^3 operations. This problem can be avoided easily through the use of the preconditioner described in [2, 10], which reduces the number of GMRES iterations required to achieve convergence with 1% error ($tol = 0.01$ in Algorithm 1) to well below n for large problems.

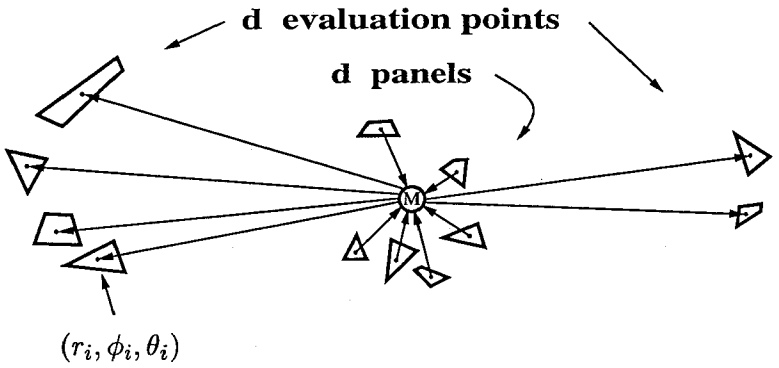

Figure 1: Approximately computing the potentials at d evaluation points due to a cluster of d charged panels in order d operations using a multipole expansion.

2.4 Multipole Acceleration

In the case of collocation, computing the dense matrix-vector product Pq is equivalent to evaluating the potential at N collocation points, $\{x_1, ..., x_N\}$, due to a charge density described by $\sum_{i=1}^{N} q_i \theta_i(x)$. It is possible to avoid forming P, and to substantially reduce the cost of computing Pq, using the fast multipole algorithm [11, 12]. The fast multipole algorithm uses a hierarchical partitioning of the problem domain and careful application of multipole and local expansions to accurately compute potentials at N points due to N charged particles in order N operations.

To understand how the fast multipole algorithm achieves this efficiency, consider again the case where the expansion functions represent uniform distributions over flat panels and centroid collocation is used to determine the coefficients of the expansion. Then evaluating the potential due to the charge distribution on d panels at d centroid collocation points, or evaluation points, requires d^2 operations. If the panels are in a cluster, then the cost of this calculation can be reduced if some approximation is allowed. The potential due to the cluster of panels can be represented by a truncated multipole expansion, and this expansion can used to compute the potential at d evaluation points, as shown in Figure 1. Multipole expansions have the general form

$$\psi(r, \theta, \phi) \approx \sum_{n=0}^{l} \sum_{m=-n}^{n} \frac{M_n^m}{r^{n+1}} Y_n^m(\theta, \phi), \tag{17}$$

where l is the expansion order; r, θ and ϕ are the spherical coordinates with respect to the multipole expansion's origin (usually the center of the charge cluster); $Y_n^m(\theta, \phi)$'s are the surface spherical harmonics; and the M_n^m's are the multipole coefficients [13].

Multipole expansions can be used to efficiently evaluate the potential due to a cluster of charges at any point where the distance between the evaluation point and the cluster's center is significantly larger than the radius of the cluster. A dual optimization is possible using local expansions, as shown in Figure 2. That is, for a cluster of evaluation points, the potential due to charges whose distances from the cluster's center are significantly larger than the radius of the cluster can be combined into a local expansion at the cluster's center. Then, this local expansion can be used to efficiently compute potentials at evaluation points in the cluster. A local expansion has the form

$$\psi(r, \theta, \phi) \approx \sum_{n=0}^{l} \sum_{m=-n}^{n} L_n^m Y_n^m(\theta, \phi) r^n, \tag{18}$$

where l is the order of the expansion; r, θ and ϕ are the spherical coordinates of the evaluation location with respect to the expansion's center; and the L_n^m's are the local expansion coefficients.

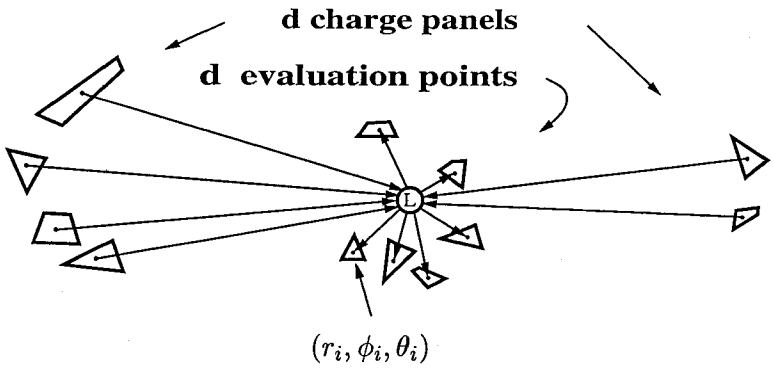

Figure 2: Approximately computing the potentials at a cluster of d evaluation points due to d charged panels in order d operations using a local expansion.

The above examples make clear that multipole and local expansions can be used to improve computational efficiency, at the cost of some accuracy, when a set of evaluation points are well-separated from a set of panel charges, and one of the sets is clustered. The loss in accuracy can be made arbitrary small by increasing the order of the multipole expansions. For a general distribution of panels, nearby interactions should therefore be computed directly. This result can then be summed with the contributions to the potential due to distant panels which, of course, can be represented using multipole or local expansions. Direct evaluations may also used for small groups of distant panels, as multipole and local expansions are inefficient unless they are used to represent the effect of a large number of panels.

3 Galerkin Formulation

In this section, we describe the formulation of the galerkin approach to the multiple dielectric problem.

We are still facing the same set of boundary constrains as given by equations (1) and (2) and trying to solve them simultaneously, and we still use the same approach to discretize both the conductor surfaces and dielectric interfaces as in the case of collocation, and still assume that on each panel i, the charge q_i on that panel, is uniformly distributed. To summarize, we can write the following expansion function to describe the charge distribution for both conductors surfaces and dielectric interfaces,

$$\sigma(x) = \sum_{i=1}^{n} \frac{q_i}{a_i} \delta_i(x), \tag{19}$$

where $\sigma(x)$ is the charge density at point x in space, q_i is the total charge on panel i, a_i is the area of panel i, $\delta_i(x)$ is one when x is in panel i, and zero otherwise. The set of $\delta_i(x)$'s forms a basis for the expansion.

The potential at any point in space can be approximated by substituting equation (19) into equation (1). We define the residual, denoted as $R(x)$, as the difference between the exact solution and the discretized solution, so the residual is

$$R(x) = \psi(x) - \sum_{j=1}^{n} \frac{q_j}{a_j} \int_{panel_j} \frac{1}{4\pi\epsilon_0 \|x_j - x\|} da_j. \tag{20}$$

The Galerkin condition requires that the expansion function to be orthogonal to the residual $R(x)$, which is also equivalent to have $\delta_i(x)$ to be orthogonal to $R(x)$ for $i = 1, 2, ..., n$.

We say that $\delta_i(x)$ is orthogonal to $R(x)$ if

$$\int_s \delta_i(x)R(x)dx = 0 \tag{21}$$

Thus, by evaluating the orthogonality equation (21) for $i = 1, 2, ..., n$, we form a similar equation as in equation (4),

$$p(x_i) = P_{i1}q_1 + P_{i2}q_2 + \cdots + P_{ij}q_j + \cdots + P_{in}q_n, \tag{22}$$

but now

$$P_{ij} \triangleq \frac{1}{a_i a_j} \int_{panel_i} \int_{panel_j} \frac{1}{\|x_i - x_j\|} da_j da_i. \tag{23}$$

Substituting (22) into (2) and we get

$$D_{i1}q_1 + D_{i2}q_2 + \cdots + D_{ij}q_j + \cdots + D_{in}q_n = 0, \tag{24}$$

where

$$D_{ij} \triangleq (\epsilon_a - \epsilon_b)\frac{\partial}{\partial n_i}\frac{1}{a_i a_j} \int_{panel\ i} \int_{panel\ j} \frac{1}{4\pi\epsilon_0\|x_i - x_j\|}\, da_j da_i, \qquad i \neq j, \tag{25}$$

and

$$D_{ii} \triangleq \frac{(\epsilon_a + \epsilon_b)}{2a_i\epsilon_0}. \tag{26}$$

To get E_{ij}, scale D_{ij} by $1/(\epsilon_a - \epsilon_b)$

$$E_{ij} \triangleq \frac{\partial}{\partial n_i}\frac{1}{a_i a_j} \int_{panel\ i} \int_{panel\ j} \frac{1}{4\pi\epsilon_0\|x_i - x_j\|}\, da_j da_i, \qquad i \neq j, \tag{27}$$

and

$$E_{ii} \triangleq \frac{(\epsilon_a + \epsilon_b)}{2a_i\epsilon_0(\epsilon_a - \epsilon_b)}. \tag{28}$$

For close panel interactions, equation (23) can be evaluated with two dimensional Gaussian quadrature in combination with the closed form expression of the inner integral [14, 15]. The number of close panel interactions can be reduced by half by realizing the fact that the $P_{ij} = P_{ji}$.

Since the inner integral of the expression (23) describes the potential at point x_i due to panel j, if panel i is far away from panel j, we can use local expansion (18) to approximate the inner integral. Therefore,

$$P_{ij} \approx \int_{panel_i} \sum_{n=0}^{l} \sum_{m=-n}^{n} r^n L_n^m Y_n^m(\theta, \phi) da_i. \tag{29}$$

After switching the summations and integral, and taking the local expansion coefficient L_n^m out of the integral,

$$P_{ij} \approx \sum_{n=0}^{l} \sum_{m=-n}^{n} L_n^m \int_{panel_i} r^n Y_n^m(\theta, \phi) da_i. \tag{30}$$

In the above equation, the integral part is actually the conjugate of the multipole expansion coefficients for panel i, and therefore we have the following formula,

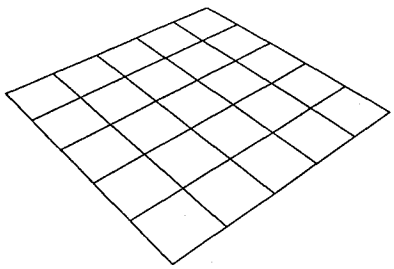

Figure 3: One plate discretized with 5x5 square panels.

$$P_{ij} \approx \sum_{n=0}^{l} \sum_{m=-n}^{n} L_n^m (M_n^m)^*. \tag{31}$$

After writing P_{ij} in terms of multipole and local expansion coefficients, the galerkin approach is easily incorporated into the multipole algorithm as described in section 2.4.

4 Preliminary results

To demonstrate the efficiency and accuracy of the Galerkin-based multipole-accelerated capacitance extraction algorithm, the capacitances associated with several test problems were computed. All the results were obtained using our Galerkin implementation of the algorithm in the program FASTCAP2, with the default 1% convergence tolerance ($tol = 0.01$ in Algorithm 1) and second-order expansions ($l = 2$ in (17) and (18)).

To demonstrate that using the Galerkin method produces more accurate capacitances for single dielectric problems, consider the comparisons in graphs (4) and (6). These graphs compare the self capacitance of a square plate (Fig. 3) and a cube (Fig. 5) calculated using collocation and the Galerkin method. The Galerkin method is somewhat better for coarse discretizations. This results agrees with [16].

The additional accuracy of the Galerkin method is much more pronounced in problems with multiple dielectrics. Fig. 7 shows two concentric spheres. The inner sphere is a conducting interface of radius 1 and outer sphere is a dielectric interface of radius 2. The outer sphere is cut to expose the inner sphere.

Fig. 8 shows the comparison of the sphere capacitance calculations with different permittivity ratios (ϵ_b/ϵ_a). It can be seen that as the permittivity ratio gets larger, the solution computed by collocation becomes quite inaccurate, but the solution computed with the galerkin is still quite accurate.

As mentioned in Section 3, Gaussian quadrature is used to compute the Galerkin integrals for nearby panels, and expansion inner products are used to compute the Galerkin integrals for panels approximated by multipole expansions. To show that the approach is not much more expensive than using collocation methods for large problems, we generated progressively larger problems by replicating a sphere problem. The results, tabulated in Table (1), show that for large problems the collocation method is only twenty percent slower than collocation, but as noted above, much more accurate.

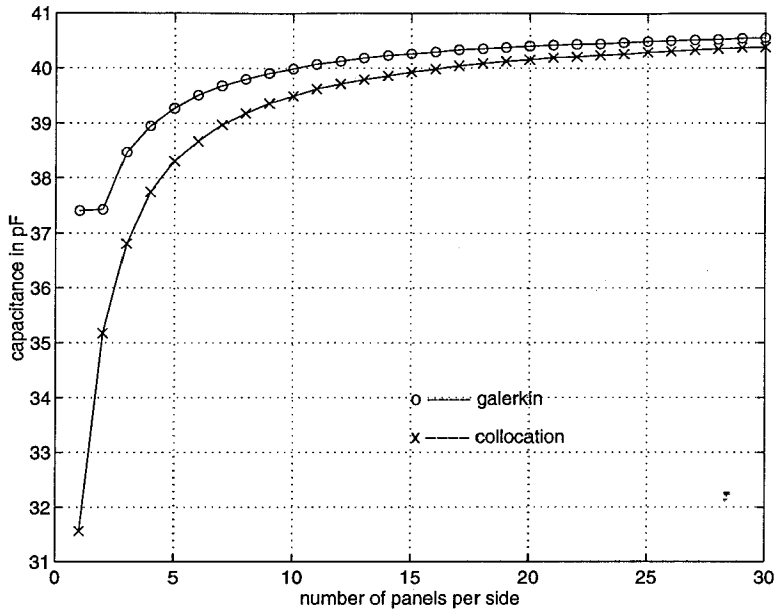

Figure 4: The self capacitance of the square plate vs. number of panels.

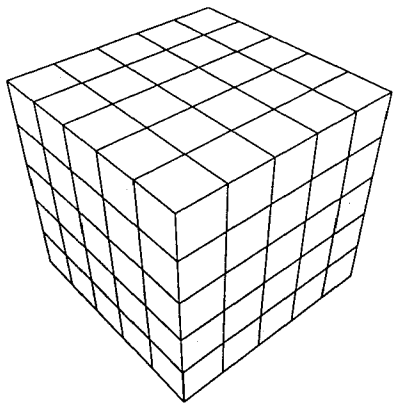

Figure 5: A cube discretized square panels.

spheres	panels	Galerkin CPU Seconds	Collocation CPU Seconds
1	1600	111.05	49.38
2	3200	275.18	145.93
3	4800	469.07	250.73
4	6400	737.740	639.960

Table 1: Comparison of CPU times for Galerkin and Collocation for problems with progressively more spheres

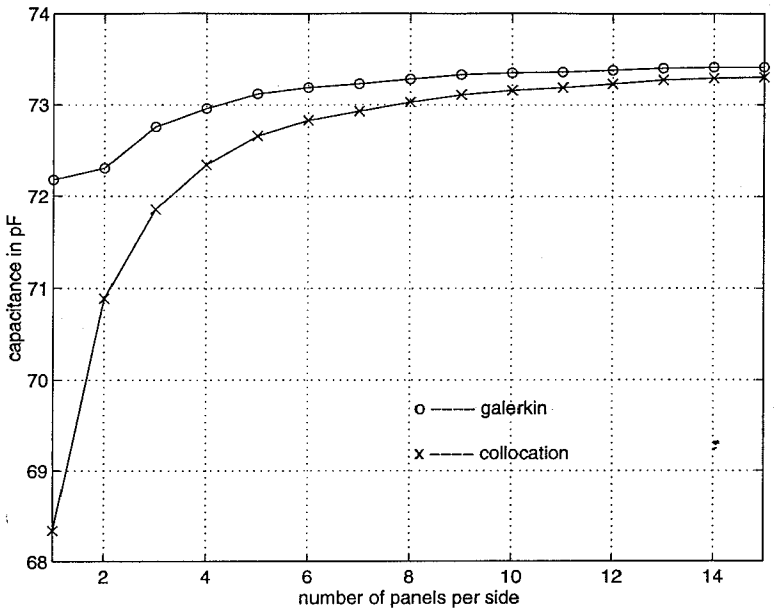

Figure 6: The self capacitance of a cube vs. number of panels.

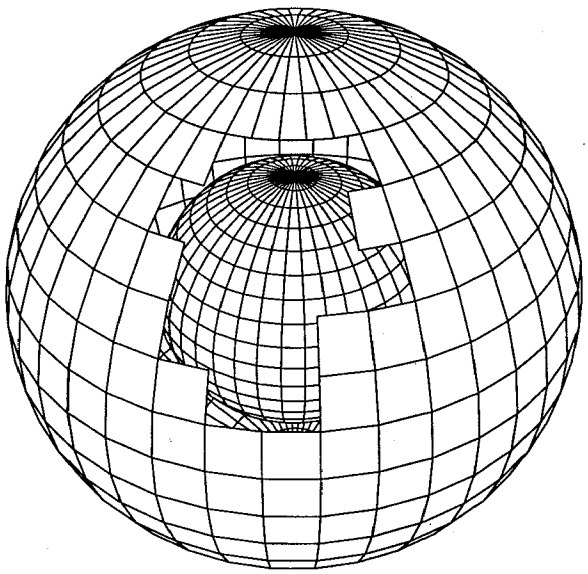

Figure 7: The dielectric sphere example. Outer sphere is cut to expose the inner one.

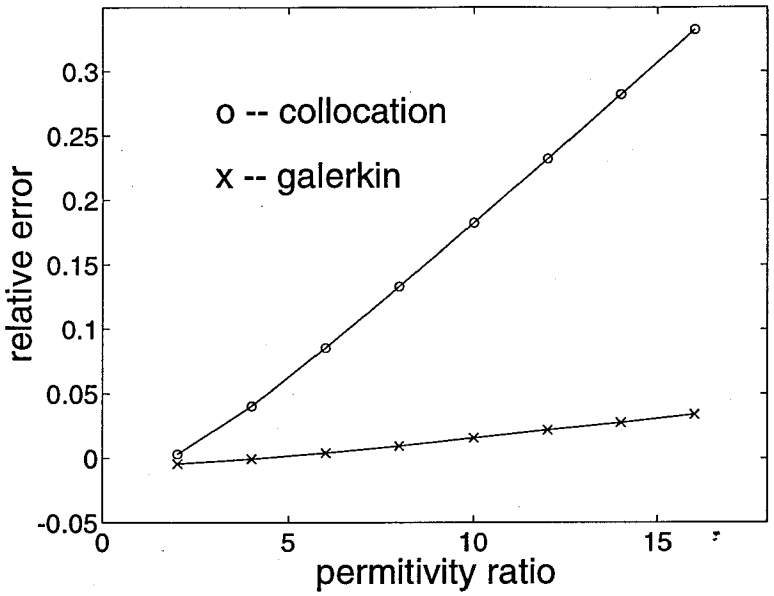

Figure 8: The comparison of dielectric calculation of different methods.

5 Conclusion

In this paper we described an efficient approach to using Galerkin methods in a multipole-accelerated capacitance extraction program. We showed that the Galerkin method is twenty percent more expensive than using collocation for a fixed discretization on large problems. In addition, we showed that for problems with widely varying dielectric constants and coarse discretizations, the Galerkin method can be thirty times more accurate.

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