Improved Integral Formulations for Fast 3-D Method-of-Moments Solvers

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***Abstract*—This paper introduces a new integral formulation to calculate charge densities of conductor systems that may include multiple dielectric materials. We show that the conditioning of our formulation is much better than that of the standard equivalent charge formulation. When combined with a nonstandard discretization scheme, results can be obtained with higher accuracy at reduced numerical cost. We present a multipole accelerated implementation of our formulation. The results demonstrate that the new approach can cut the iteration count by a factor between two and four. Moreover, we will demonstrate that in the presence of sparsification errors and multiple dielectric materials second-kind formulations are much more accurate than the standard first-kind formulations.**

***Index Terms*—Boundary-element methods, capacitance, dielectric materials.**

I. Introduction

FOR THE design of high-performance very large scale integration (VLSI) circuits and integrated circuit packaging, it is important to obtain accurate estimates of the capacitances of complicated three-dimensional conductor systems that often include multiple dielectric materials with high permittivity ratios. The commonly used algorithms in electrostatics are based on boundary integral reformulations of Laplace's equation and are collocation, i.e., method of moments [4] or Galerkin [17] discretizations of the single-layer potential.

These methods generate dense and ill-conditioned matrix problems which severely limit the complexity of the structures that can be analyzed, even with today's computing hardware. Since iterative methods, such as generalized minimal residual algorithms (GMRES), are usually employed, the problem is that a large vector must be applied to a large matrix a large number of times.

The main thrust of research in the past decade has been to develop techniques to accelerate the matrix-vector product. These methods are based on the fast multipole method [3], [10], the fast Fourier transform [13], singular value decomposition [6], multiscale [21], and dimension-reduction ideas [5].

All the above papers describe algorithms for the single-layer equation, which is an integral equation of the first kind and, therefore, ill-conditioned. The conditioning effects the performance of the algorithms in two negative ways. First, iterative methods converge slowly. Second, small errors introduced by accelerated matrix-vector products can be magnified. While the preconditioners described in [10], [21], and [22] can accelerate the speed of iterative solvers, the sensitivity of the error is inherent to the integral formulation.

The presence of multiple dielectric materials complicates matters further. In this case, the first-kind equation on the conductor surfaces must be supplemented with a second-kind equation on the dielectric interfaces. The resulting formulation is also known as the equivalent charge formulation (ECF) [14]. A typical conductor system with dielectrics requires more iterations to converge than a comparable structure without dielectrics. When the ratio of the permittivities is large, e.g., on the order of ten, then the accuracy of the approximation becomes poor and perturbation techniques must be employed [20].

It is known that second-kind integral equations result in well-conditioned linear systems, but the standard second-kind formulation in potential theory is based on the dipole potential, which is of limited use for circuit parameter extraction and cannot be generalized to multiple dielectric materials. In [19], we have introduced a new second-kind formulation for the charge density for the single dielectric case and proved that it is well posed. The purpose of this paper is to discuss issues associated with the discretization and multipole acceleration. Moreover, we will present a new extension to multiple dielectric materials, which is purely second-kind as opposed to the mixed first-second-kind ECF. We will conclude with comparisons of accuracy and efficiency of this approach and existing approaches.

II. Standard Formulations

In this section, we briefly review the standard integral formulations that have been used extensively to calculate capacitances of complex multiconductor systems. However, since they are of the first kind on the conductor surfaces, they lead to ill-conditioned linear systems.

Under the electrostatic assumption, the electric field has a potential ϕ, which satisfies Laplace's equation. In an M-conductor

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system, where the kth conductor has potential p_k, the potential satisfies a Dirichlet boundary condition of the form

$$\phi(x) = f(x) := \sum_{k=1}^{M} p_k \chi_k(x), \quad x \in S_c \tag{1}$$

where $S_c = S_1 \cup \cdots \cup S_M$ denotes the collection of all conductor surfaces S_k and χ_k is the characteristic function of the kth conductor given by

$$\chi_k(x) = \begin{cases} 1, & x \in S_k \\ 0, & \text{elsewhere.} \end{cases} \tag{2}$$

If, in addition to the conductors, dielectric media with different permittivities are present, then the flux condition

$$\varepsilon^+ \frac{\partial \phi}{\partial n}^+ (x) = \varepsilon^- \frac{\partial \phi}{\partial n}^- (x), \quad x \in S_d \tag{3}$$

must be imposed on the interface S_d of two dielectrics. Here, ε^+ is the permittivity in the direction of the surface normal n and ε^- is the permittivity in the opposite direction. Note that we have normalized the problem by letting the vacuum permittivity $\varepsilon_0 = 1$.

The conductor charge can be calculated by the ECF [11], [14], [16]. In this formulation, surface charge layers with densities σ_c and σ_d are placed on the conductor surfaces as well as dielectric interfaces. This results in the electrostatic potential

$$\phi(x) = \mathcal{V}_c \sigma_c(x) + \mathcal{V}_d \sigma_d(x), \quad x \in \mathbf{R}^3. \tag{4}$$

Here, $\mathcal{V}_c$ and $\mathcal{V}_d$ denote the single-layer potentials due to charges on S_c and S_d, respectively, which are given by

$$\mathcal{V}_a \sigma(x) = \int_{S_a} G(x, x') \sigma_a(x') \, dS_{x'}, \quad x \in \mathbf{R}^3$$

where $a \in \{c, d\}$. The kernel $G(x, x')$ is the free-space Green's function for the Laplace operator in three dimensions

$$G(x, x') = \frac{1}{4\pi} \frac{1}{|x - x'|}. \tag{5}$$

The single-layer potential must satisfy the Dirichlet condition on the conductor surfaces as well as the flux condition on the dielectric interfaces. These conditions will lead to a system of integral equations for the unknown densities σ_c and σ_d.

To better understand the derivation of this system, we recall the limiting values of the single-layer potential for $x \to S$; the details can be found in most texts on potential theory, e.g., [7]. The single-layer potential is continuous as the field point approaches the surfaces. On the other hand, its normal derivative has different values on either side of the surface and satisfies the jump relation

$$\frac{\partial \phi}{\partial n}^{\pm} (x) = \mp \frac{1}{2} \sigma_d(x) + \mathcal{K}'_c \sigma_c(x) + \mathcal{K}'_d \sigma_d(x), \quad x \in S_d. \tag{6}$$

Here, $\mathcal{K}'_a$ denotes the adjoint of the double-layer operator, which is given by

$$\mathcal{K}'_a \sigma_a(x) = \int_{S_a} \frac{\partial}{\partial n_x} G(x, x') \sigma_a(x') \, dS_{x'}$$

for $a \in \{c, d\}$. Combining (4) and (6) with the boundary conditions (1) and (3), the following system of integral equations for the densities σ_c and σ_d can be derived:

$$\begin{aligned} \mathcal{V}_{cc} \sigma_c + \mathcal{V}_{cd} \sigma_d &= f \\ \mathcal{K}'_{dc} \sigma_c + \left(\frac{1}{2\lambda} + \mathcal{K}'_{dd} \right) \sigma_d &= 0 \end{aligned} \tag{7}$$

where the subscript ab denotes a potential due to a charge on surface b evaluated at surface a. The parameter λ depends on the permittivities on both sides of the dielectric interface via the relation

$$\lambda = \frac{\varepsilon^- - \varepsilon^+}{\varepsilon^- + \varepsilon^+}. \tag{8}$$

If there is only one dielectric material present, the potential is generated only by conductor charges. In this case, integral equation (7) reduces to

$$\mathcal{V}_{cc} \sigma_c = f \tag{9}$$

which is usually referred to as the single-layer equation.

III. Second-Kind Formulations

Many difficulties associated with the first-kind formulation can be avoided by using a second-kind integral formulation for Laplace's equation. Typically, the arising integral equations and their discretizations are well conditioned. Hence, they do not magnify sparsification errors and iterative solvers require fewer iterations to converge.

The capacitance problem is an exterior Dirichlet problem for the Laplace equation. Using double-layer potentials, this problem can be cast into a second-kind integral equation. The resulting operator has an M-dimensional nullspace, which can be removed by augmenting the integral equation with M Lagrange multipliers (see [1] and [8]). The multipliers turn out to be the capacitances.

However, double-layer potentials do not directly yield the charge density as a function on the conductors. In multiple dielectric case, this approach is much harder to implement because hypersingular integral operators arise, which require higher order discretizations. In [19], we have already introduced a well-conditioned second-kind formulation in which the charge density is solved directly for the single-dielectric case. In Section III-A, we will briefly review this formulation and describe the novel modifications to handle multiple dielectric materials.

A. Single Dielectric Case

Since the potential ϕ is constant on each conductor surface, it follows that ϕ is also constant in the interior of each conductor and, hence, the gradient vanishes on the conductor surfaces when approached from the inside. From the jump relation of the normal derivative of the single-layer potential (6), it then follows that

$$(1/2 + \mathcal{K}'_{cc}) \sigma_c = 0. \tag{10}$$

Integral equation (10) is singular because any charge distribution that generates a constant potential on the conductor surfaces will solve it. To determine σ uniquely, the potential must be fixed for each conductor. This can be achieved by imposing that the potential satisfies

$$\mathcal{V}_c\sigma_c(x_k) = p_k, \quad k = 1, \ldots, M \tag{11}$$

where x_k is a point in the *interior* of conductor k.

Integral equation (10) combined with condition (11) is a system with more equations than unknowns. Without changing the solution, (10) and (11) can be combined to the well-posed integral equation

$$\left(\frac{1}{2} + \mathcal{K}'_{cc} + \mathcal{A}_c\mathcal{G}'_c\right)\sigma_c = \mathcal{A}_c p \tag{12}$$

where the operators $\mathcal{A}_c$ and $\mathcal{G}'_c$ are defined by

$$\mathcal{A}_c p(x) = \sum_{k=1}^{M} \frac{p_k}{\sqrt{|S_k|}}\chi_k(x), \quad x \in S_c \tag{13}$$

$$[\mathcal{G}'_c\sigma_c]_k = \int_{S_c} G(x_k, y)\sigma_c(y)\, dS_y \tag{14}$$

where $|S_k|$ is the surface area of conductor k. Note that the operator $\mathcal{A}_c$ maps an M vector onto a function that is constant on each conductor surface, whereas $\mathcal{G}'_c$ maps a function on the conductors on an M vector.

The key to understand why the solution of (12) is also the solution of (9) is the observation that the range of the operator $1/2 + \mathcal{K}'_{cc}$ is orthogonal to the functions which are constant on each conductor. This is a simple consequence of Gauss' Law (see, e.g., [8]). Thus, for the solution of (12)

$$\left(\frac{1}{2} + \mathcal{K}'_{cc}\right)\sigma_c + \mathcal{A}_c(\mathcal{G}'_c\sigma_c - p) = 0$$

it follows from the orthogonality of the ranges of $(1/2 + \mathcal{K}'_{cc})$ and $\mathcal{A}_c$ that both vectors in the above sum must vanish and, therefore, (10) and (11) must hold.

By the same token, for any nonsingular $M \times M$ matrix B, the solution of integral equation

$$\left(\frac{1}{2} + \mathcal{K}'_{cc} + \mathcal{A}_c B\mathcal{G}'_c\right)\sigma_c = \mathcal{A}_c B p \tag{15}$$

is well posed and provides the solution of the capacitance problem. The matrix B plays the role of a preconditioner.

B. Extension to Multiple Dielectrics

The ECF (7) can be converted into a purely second-kind system in a similar fashion as the single-layer equation. As in the single-dielectric case, the potential must be constant inside the conductors and hence the normal derivative on the conductor surfaces approached from the inside must vanish. Thus, on the conductor surfaces we have

$$(1/2 + \mathcal{K}'_{cc})\sigma_c + \mathcal{K}'_{cd}\sigma_d = 0. \tag{16}$$

Equation (16) must be supplemented with the flux condition on the dielectric interfaces, which is the same as in the ECF

$$\mathcal{K}'_{dc}\sigma_c + \left(\frac{1}{2\lambda} + \mathcal{K}'_{dd}\right)\sigma_d = 0. \tag{17}$$

The latter two equations constitute a system for the unknown charges σ_c and σ_d, which is singular because any charge that generates constant potentials on each conductor will solve it. In order to determine the charge uniquely, the potentials must be specified at points x_k, which are interior to conductor k.

$$\mathcal{V}_c\sigma_c(x_k) + \mathcal{V}_d\sigma_d(x_k) = p_k, \quad k = 1, \ldots, M. \tag{18}$$

Equations (16)–(18) are an overdetermined system. To obtain a well-posed problem, we combine (16) and (18) in a similar manner as for the single dielectric case. The resulting system has the form

$$\left(\frac{1}{2} + \mathcal{K}'_{cc}\right)\sigma_c + \mathcal{K}'_{cd}\sigma_d + \mathcal{A}_c B\mathcal{G}'_c\sigma_c + \mathcal{A}_c B\mathcal{G}'_d\sigma_d = \mathcal{A}_c B p$$

$$\mathcal{K}'_{dc}\sigma_c + \left(\frac{1}{2\lambda} + \mathcal{K}'_{dd}\right)\sigma_d = 0 \tag{19}$$

where B is any nonsingular $M \times M$ matrix. We will also write the integral equation more compactly as

$$(\Lambda + \mathcal{K}' + \mathcal{A}_c B\mathcal{G}')\sigma = \mathcal{A}_c B p \tag{20}$$

where $\Lambda = \mathrm{diag}(1/2, 1/(2\lambda))$ and $\sigma, \mathcal{K}', \mathcal{G}'$ are quantities defined on both surfaces. The operator $\mathcal{A}_c$ is defined for the conductor surfaces in (13) and vanishes on the dielectric interface.

IV. Discretization of the Adjoint Operator

The single-layer potential in the first-kind formulation represents the potential due to a surface charge distribution, which always remains finite. On the other hand, the adjoint operator in the second-kind integral formulations is the normal derivative of the potential, which can become infinite near possible edges of the surface. Thus, integral equations (15) and (20) require special care for their discretization.

Furthermore, the second-kind integral formulations rely on the orthogonality of the range of $(1/2) + \mathcal{K}'$ to the constant functions. To obtain accurate results, this property must be preserved when this operator is discretized.

The Galerkin method can handle both difficulties. However, in its pure form, this scheme cannot be realized because the coefficients of the discretization matrix involve integrals that cannot be computed exactly, except in special cases [16]. On the other hand, the collocation method has closed-form integrals, but has problems with singularities and orthogonality.

In the following two paragraphs, we will discuss these issues in more detail and propose a qualocation scheme that has closed-form integrals and the same stability properties as the Galerkin method.

1) Collocation Versus Qualocation: Consider a discretization of the conductor surfaces and dielectric interfaces into N triangular or quadrilateral panels P_i. The Galerkin method seeks a solution as a piecewise constant function on this subdivision and enforces the integral equation by integration over the panels.

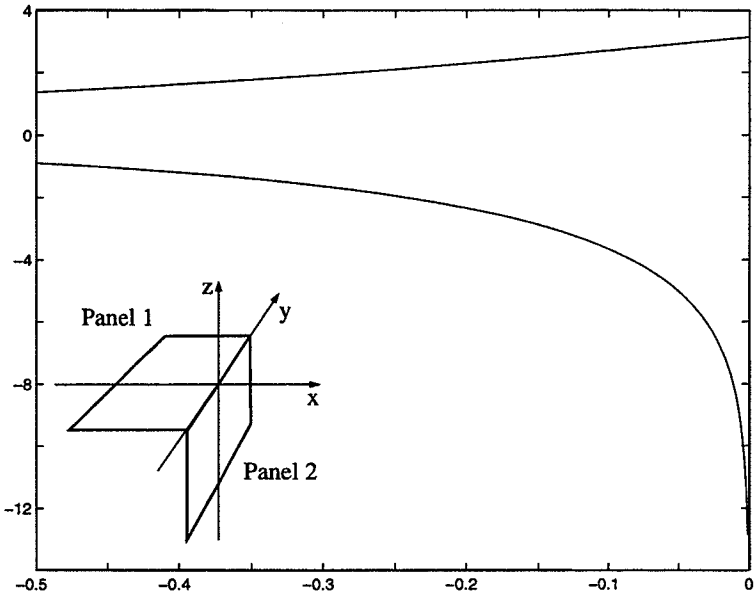


Fig. 1. Dipole potential due to Panel 2 evaluated at the x axis (top curve) and normal derivative of source potential due to Panel 1 evaluated at the z axis (bottom curve).

This leads to a linear system whose coefficients contain entries of the form

$$K_{\text{gal}}(i,j) = \int_{P_i}\int_{P_j} \frac{\partial}{\partial n_x} G(x,y)\, dS_y\, dS_x. \tag{21}$$

For panels in general position, there are no closed-form expression for the double integrals and, therefore, numerical quadrature schemes must be applied. For efficiency reasons, simple quadrature schemes are desirable. The most commonly used scheme is the collocation discretization, which in this context can be regarded as replacing the integration over panel P_i in (21) by the midpoint quadrature rule. Thus, a matrix entry is of the form

$$K_{\text{col}}(i,j) = \alpha_i \int_{P_j} \frac{\partial}{\partial n_i} G(\xi_i, y)\, dS_y \tag{22}$$

where ξ_i denotes the centroid of panel P_i and α_i is the area of P_i. The integral in (22) is the normal derivative of the source potential due to panel P_j evaluated at the point ξ_i. This scheme is popular because the integral over P_j has a closed-form expression, see, e.g., Newman [12]. Note, that in the collocation method the factor α_i cancels.

An alternative scheme that can be derived from the Galerkin method is is the qualocation scheme, which replaces the integration over panel P_j in (21) by midpoint quadrature. The resulting matrix entries are of the form

$$K_{\text{qal}}(i,j) = \int_{P_i} \frac{\partial}{\partial n_i} G(x,\xi_j)\, dS_x\, \alpha_j \tag{23}$$

and may be regarded (up to the factor α_j) as the dipole potential due to panel P_j evaluated at ξ_i.

The choice of the panel where integration is replaced by quadrature has a significant effect on the accuracy. It is known (see, e.g., Michlin [9]) that the dipole potential due to P_i is a solid angle that remains bounded over P_j even if the panels are equal or adjacent. On the other hand, the gradient of the source potential due to P_i becomes infinite at common edges of adjacent panels. This effect is illustrated in Fig. 1. Qualocation has superior accuracy over collocation because the singular integral is evaluated analytically and the smooth integral is evaluated with midpoint quadrature.

2) Qualocation Preserves the Correct Range: The fundamental principle behind the second-kind formulations in the single- and the multiple-dielectrics case is the orthogonality of the ranges of $(\Lambda + \mathcal{K}')$ and $\mathcal{A}_c\mathcal{G}'$. The latter range consists of functions that are constant on each conductor. It is important that the discretized system also preserves this orthogonality relation and we will demonstrate below that qualocation has this property whereas collocation does not.

To better understand the conservation of orthogonality, let us consider the dipole operator on $S = S_c \cup S_d$

$$\mathcal{K}\mu(x) = \int_S \frac{\partial}{\partial n_y} G(x,y)\mu(y)\, dS_y, \quad x \in S \tag{24}$$

which is the adjoint of $\mathcal{K}'$. Because the nullspace is always the orthogonal complement of the range of the adjoint, we see that

$$\mathcal{N}(\Lambda + \mathcal{K}) = \mathcal{R}(\Lambda + \mathcal{K}')^{\perp} = \text{span}[\chi_1, \ldots, \chi_M]. \tag{25}$$

Let K_{dip} be the matrix obtained from collocation discretization of $\mathcal{K}$ using the same partition into panels as for the adjoint operator. The matrix entries are given by

$$K_{\text{dip}}(i,j) = \int_{P_j} \frac{\partial}{\partial n_j} G(\xi_i, y)\, dS_y. \tag{26}$$

It is follows that the qualocation matrix of the adjoint operator in (23) is the transpose of the collocation matrix of the dipole operator except for a factor of area

$$K_{\text{qal}} = K_{\text{dip}}^T D \tag{27}$$

where $D = \mathrm{diag}(\alpha_1, \ldots, \alpha_N)$. Furthermore, if $\chi_{k,N}$ denotes the vector that is unity on the nodes corresponding to conductor k and zero elsewhere, then we see from (25) and (26) that

$$\mathcal{N}(\Lambda + K_{\mathrm{dip}}) = \mathcal{R}(\Lambda + K_{\mathrm{qal}})^{\perp} = \mathrm{span}[\chi_{1,N}, \ldots, \chi_{M,N}]. \tag{28}$$

For the collocation discretization of the adjoint operator K_{col}, there is no relationship to K_{dip} similar to (27) and, in general, the nullspace of $\Lambda + K_{\mathrm{col}}$ does not consist of the $\chi_{k,N}$'s.

The importance of a discretization that preserves orthogonality of the ranges becomes apparent when looking at the qualocation discretization of the second-kind formulations. For both the single and the multiple dielectrics case, the discretization assumes the form

$$\left(\Lambda + K_{\mathrm{qal}} + A_N B G_N^T\right) D\sigma_N = A_N B p \tag{29}$$

where A_N and G_N are discretizations of $\mathcal{A}_c$ and $\mathcal{G}$, respectively. Since

$$\mathcal{R}(A_N) = \mathrm{span}[\chi_{1,N}, \ldots, \chi_{M,N}]$$

it follows again from orthogonality that for the solution σ_N of (29)

$$(\Lambda + K_{\mathrm{qal}}) D\sigma_N = 0$$

and

$$G_N' D\sigma_N = p.$$

Thus, σ_N satisfies the discretizations of the Neumann boundary condition (10) as well as the condition on the potential (11) [(16) and (18) in the multiple dielectrics case]. Furthermore, the qualocation solution is independent of the matrix B and, hence, B can be chosen solely based on improving iterative method convergence.

V. Numerical Results

To demonstrate the differences between the integral formulations described in this article, we compute the charge densities and capacitances of some structures in homogeneous and multiple dielectric materials. The formulations tested are:

1) collocation discretization of the single-layer equation (9) and the ECF (7);
2) collocation discretization of the second-kind formulations (15) and (19);
3) qualocation discretization of formulations (15) and (19);
4) Galerkin discretization of the ECF;
5) perturbation approach for the ECF [20].

The discretized linear systems are solved using the iterative solver GMRES [18]. For all examples, the iteration was continued until the residual was reduced by the factor 10^{-9}. No preconditioner in the usual sense was used for any calculation. However, the iteration counts of the second-kind formulations are somewhat dependent on the choice of the matrix B in (15) and (19) and B can be regarded as an inexpensive method to improve the performance of iterative solver for second-kind formulations. In our experiments, we set $B = (\mathcal{G}_c' \mathcal{A}_c)^{-1}$, where $\mathcal{A}_c$ and $\mathcal{G}_c'$ are defined in (13) and (14). With this choice of B, the eigenvalues of $\mathcal{A}_c B \mathcal{G}_c'$ are all unity or zero, which implies that the eigenvalues of $\Lambda + \mathcal{K}'$ are not changed much by adding $\mathcal{A}_c B \mathcal{G}_c'$.

TABLE I
Maximum Errors of the Charge Density When Refining the Mesh

Panels	1st colloc	2nd colloc	2nd qualoc
196	0.2446	0.3828	0.3104
768	0.1336	0.2510	0.1591
3,072	0.0765	0.1595	0.0908
12,288	0.0405	0.0884	0.0441
49,152	0.0289	0.0550	0.0214

Ellipsoid in homogeneous medium with multipole acceleration. The maximum of the exact solution is $0.98\ldots$.

To accelerate the matrix-vector products, the fast multipole algorithm (FMM) was applied [3], [15]. Our code is based on the package FASTCAP [10] with some modifications to calculate matrix-vector products with the adjoint operator.

The convergence behavior of the discretization error is investigated using a single conductor with ellipsoidal geometry

$$S_c = \left\{ x \in \mathbf{R}^3 : \frac{x_1^2}{4} + \frac{x_2^2}{1} + \frac{x_3^2}{9} = 1 \right\}$$

where, for examples with dielectrics, the interface

$$S_d = \left\{ x \in \mathbf{R}^3 : \frac{x_1^2}{5} + \frac{x_2^2}{2} + \frac{x_3^2}{10} = 1 \right\}$$

is added. For both geometries with and without dielectrics, the charge density can be expressed in closed form in terms of ellipsoidal coordinates [7].

Table I compares the maximum error $\max |\sigma_{\mathrm{exact}} - \sigma_{\mathrm{comput}}|$ of the numerical solution for a conductor in free space when the discretization is uniformly refined. The convergence rate with respect to refining the meshsize appears to be of order one for all discretization methods, but the constant factor of the first-kind formulation and the qualocation discretization is smaller than that of collocation for the second-kind formulation.

Matrix sparsification techniques, such as the FMM, contribute an additional error to the discretization error because far-field interactions are approximated by truncated multipole expansions. Because of better conditioning, the second-kind formulations are much less sensitive to the sparsification error than the first-kind formulation. This is demonstrated in Table II. In this example, second-kind qualocation is five times more accurate than first-kind collocation when order-two multipole expansions are used. Thus, the second-kind formulation permits lower expansion orders and, therefore, produces results of the same accuracy at reduced computational cost.

When multiple dielectric materials are present, the accuracy of standard methods deteriorates. On the other hand, second-kind qualocation maintains order one convergence

TABLE II
MULTIPOLE SPARSIFICATION ERRORS OF THE CHARGE DENSITY

order	1st colloc	2nd colloc	2nd qualoc
0	11.7226	0.7880	0.7842
1	1.2039	0.1937	0.1796
2	0.1976	0.0698	0.0373
3	0.0503	0.0565	0.0229
4	0.0278	0.0550	0.0214
5	0.0292	0.0550	0.0216
6	0.0289	0.0550	0.0214

Ellipsoid without dielectric interface. 49 152 panels. The maximum of the exact solution is 0.98 ....

TABLE III
MAXIMUM ERRORS OF THE CHARGE DENSITY FOR THE TWO-ELLIPSOID EXAMPLE WHEN REFINING THE DISCRETIZATION MESH

Panels	1st colloc	2nd colloc	2nd qualoc
96	0.5945	0.3299	0.1833
384	0.4813	0.3040	0.3577
1536	0.4094	0.2078	0.1531
6144	0.2649	0.1684	0.0865
24576	0.2100	0.1097	0.0498

$\varepsilon_1/\varepsilon_0 = 10$ and using multipole acceleration. The maximum of the exact solution is 1.11 ....

when refining the mesh, as evidenced in Table III for permittivity ratio ten.

It is well known that the the accuracy of the numerical solution deteriorates if the ratio of the permittivities is increased. Several approaches have been proposed to remedy this effect, for instance, using Galerkin discretization of the ECF [2] or the perturbation approach. For the two-ellipsoid structure, Table IV compares the accuracy of these approaches with the formulations described in this paper.

For the perturbation approach, the error of the charge density can be shown to be independent of ε, whereas the error of all other formulations increase with ε. Thus, for materials with large permittivity contrasts, the perturbation is the most accurate way to calculate the charge density. However, perturbation involves solving two problems consecutively, where the input of the second problem depends on the output of the first. This is why for low ε, the error of the perturbation method is larger than for the first-kind and the second-kind qualocation formulation. For the two-ellipsoid structure, the crossover occurs near $\varepsilon = 10$.

Since the *capacitance* is an integrated quantity, errors of the charge density can be cancelled under certain circumstances and, thus, a somewhat different picture emerges. As expected, the error of the capacitance calculated by the perturbation approach is independent of ε. However, if the matrix coefficients are integrated exactly and if the discretized linear system is solved exactly, Galerkin discretization of the ECF and qualocation of the second-kind formulation are also ε independent.

TABLE IV
RESULTS FOR THE TWO-ELLIPSOID EXAMPLE WHEN INCREASING THE PERMITTIVITY OF THE DIELECTRIC

$\varepsilon_1/\varepsilon_0$	2	5	10	50	100	1000
	Maximum error on conductor surface					
1st colloc	0.0427	0.1363	0.4083	2.6608	5.4866	56.370
1st Galerkin	0.0313	0.0488	0.1395	0.8846	1.8188	18.639
2nd colloc	0.1560	0.0633	0.2140	2.0076	4.2542	44.944
2nd qualoc	0.0762	0.0943	0.1493	0.6956	1.4941	15.868
perturbation	0.0964	0.1255	0.1365	0.1459	0.1471	0.1483
	Error of capacitance					
1st colloc	0.1045	2.1010	5.8906	37.125	76.288	781.45
1st Galerkin	0.1173	0.1593	0.6887	5.0607	10.544	109.27
2nd colloc	0.1162	1.9714	5.7867	36.978	76.055	779.60
2nd qualoc	0.1913	0.1784	0.1733	0.1690	0.1684	0.1672
perturbation	0.6652	0.9972	1.1178	1.2180	1.2308	1.2424

1536 panels. No multipole acceleration. The maxima of the exact values for the charge density are between 1.04 and 1.12, the exact capacitances are between 26.95 and 28.24.

TABLE V
GMRES ITERATION COUNT FOR THE ELLIPSOID

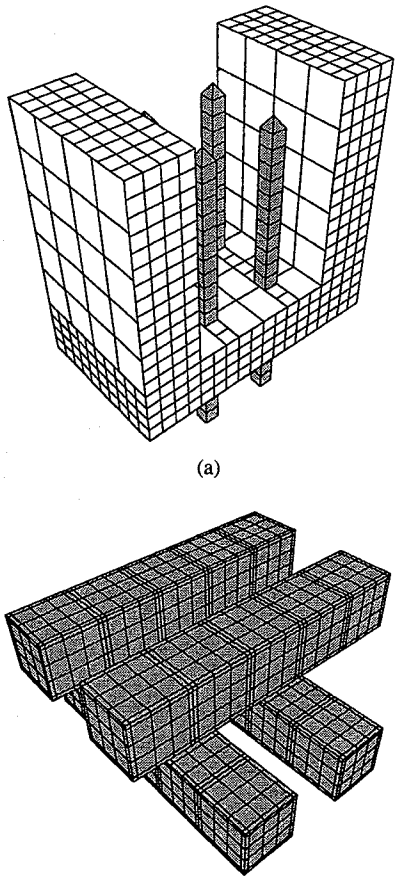
constant ε				$\varepsilon_1/\varepsilon_0 = 10$			
Panels	1st colloc	2nd colloc	2nd qualoc	Panels	1st colloc	2nd colloc	2nd qualoc
48	6	6	6	96	12	12	12
196	21	11	12	384	37	18	17
768	27	11	12	1,536	46	18	15
3,072	35	11	11	6,144	59	18	16
12,288	46	11	11	24,576	77	19	17

In a real calculation, the matrix coefficients of the Galerkin method must be approximated, whereas for qualocation, exact formulas exist. Thus, in Table IV, the errors of the capacitance increase for the Galerkin method and remain bounded for qualocation. Note that no multipole acceleration has been used for this table. In the presence of sparsification errors only the perturbation method gives accurate results for very large ε.

Due to the fact that second-kind integral formulations lead to well-conditioned linear systems, the number of GMRES iterations remains bounded when refining the discretization. On the other hand, for the first-kind formulation, the iteration count goes up with refining the mesh, as can be seen in Table V.

To demonstrate that the second-kind formulations are also useful for realistic complex multiconductor systems, we calculate the capacitance matrix associated with the bus-crossing structure and the backplane connector shown in Fig. 2. The capacitances obtained from the formulations as well as the iteration counts are displayed in Tables VI and VII.

For the bus crossing, the capacitances of the second-kind qualocation discretization are within very close agreement to the first-kind formulation at half the cost of solving the linear system. The second-kind collocation results appear to have a



(a) (b)

Fig. 2. (a) Backplane connector and (b) bus crossing. Discretization used in the calculations is finer than shown.

TABLE VI
COUPLING CAPACITANCES FOR ONE PIN AND ITERATION COUNTS FOR THE 2×2 BUS CROSSING STRUCTURE

Panels	1st colloc		2nd colloc		2nd qualoc	
its	62	80	29	31	31	32
C_{11}	28.01	28.04	26.54	27.19	27.85	27.99
C_{12}	-9.61	-9.62	-8.89	-9.19	-9.52	-9.59
C_{13}	-5.48	-5.49	-5.24	-5.36	-5.45	-5.48
C_{14}	-5.48	-5.49	-5.24	-5.35	-5.45	-5.48

Coarse grid (left), fine grid (right).

larger error, making clear that the adjoint operator requires the nonstandard qualocation discretization.

The discretization of the connector shown in Fig. 2 has been refined uniformly three times. The capacitances using these four grids are presented in Table VII. The exact value of the net-charge on each pin apears to be between 31 and 32. Collocation of the ECF largely overestimates charge densities when high-ε dielectrics are present, especially for coarse discretizations. We have seen in the ellipsoid example that the discretization error of the capacitance in the second-kind qualocation formulation does not show this behavior. However, in the connector example, matrix sparsification schemes are used and the additional error from the fast method also depends on ε, though much less than the first-kind formulations. For comparison the table includes

TABLE VII
NET CHARGES ON THE PINS WHEN THE POTENTIAL AT EACH PIN IS 1 V

	1st colloc				2nd colloc			
its	32	42	56	74	27	33	41	50
C_1	35.78	34.36	33.42	32.93	33.23	31.68	31.36	31.34
C_2	35.81	34.37	33.44	32.91	33.26	31.66	31.25	31.25
C_3	35.81	34.39	33.45	32.92	33.23	31.74	31.27	31.28
C_4	35.85	34.40	33.46	32.91	33.26	31.78	31.33	31.30
	2nd qualoc				perturbation			
its	25	27	28	28	34	47	64	74
C_1	31.39	31.76	31.89	32.03	27.54	28.96	29.98	30.61
C_2	31.39	31.70	31.85	31.95	27.56	28.95	29.96	30.61
C_3	31.39	31.72	31.90	31.95	27.52	28.97	29.99	30.61
C_4	31.41	31.73	31.92	31.98	27.54	28.96	29.96	30.61

Connector example. Three uniform refinements $\varepsilon_1/\varepsilon_0 = 10$.

the capacitances of the perturbation method. Note that the numbers are slightly different from the previously published results in [20] because here a uniform discretization has been used.

VI. CONCLUSION

We have discussed a new second-kind integral formulation for the calculation of conductor systems that may involve multiple dielectric materials. Combined with qualocation discretization, this formulation results in better approximations of charge density and capacitance at reduced cost. The gain of accuracy is most dramatic when the permittivity ratio is in the order of ten.

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