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Space and Surface Charge Excitation of a Slanted Dielectric Interface Between Two Electrodes

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David B. Seidel, Catherine L. Levinson

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Space and Surface Charge Excitation of a Slanted
Dielectric Interface Between Two Electrodes

D. B. Seidel and C. L. Levinson
Plasma Theory Division 1241
Sandia National Laboratories
Albuquerque, New Mexico 87185

ABSTRACT

The two-dimensional, electrostatic problem of a planar dielectric interface between two perfectly conducting plates has been solved numerically. The solution allows for an arbitrary interface angle relative to the plates as well as arbitrary distributions of both charge within the volume and surface charge along the interface. The problem is treated by first converting the governing differential equations to a pair of coupled integral equations using Green's function techniques, then solving these integral equations numerically using moment methods. This report details this solution and shows some sample results. This work was motivated by the need to understand the physics of dielectric breakdown by flashover in high voltage insulator applications. Of particular interest is the physics associated with Magnetic Flashover Inhibition (MFI), a possible method of significantly increasing insulator breakdown strength above that possible using currently proven technologies. A solution of this type has several apparent advantages over existing techniques for treating this type of problem and is currently being adapted for use in an existing two-dimensional Particle-In-Cell (PIC) code.

I. INTRODUCTION

One of the major impediments to increasing the power density in pulsed power drivers is the power density limitation imposed by a conventionally graded dielectric vacuum insulator. To increase this power density limit, Magnetic Flashover Inhibition (MFI) has been developed.¹ MFI refers to the structuring of the electric and magnetic fields near the vacuum/dielectric interface in such a way that electrons will $\vec{E} \times \vec{B}$ drift away from the insulator. This consequently inhibits secondary electron emission from the insulator surface, which is believed to be an important factor leading to insulator flashover. Previous theoretical work on this subject^{2,3} has been one-dimensional and has used single particle trajectories. Recently, a 2-D steady-state particle-in-cell (PIC) code⁴ has been modified to treat this problem.⁵

The work described in this report was originally conceived as a method of verifying by a different technique the field-solving algorithm in the 2-D PIC code. It has since evolved into an interesting possibility for use as the field solving algorithm for the 2-D PIC code for MFI.⁵ Rather than using finite difference techniques, it relies upon use of Green's functions and Green's integral theorem to obtain coupled integral equations for the potential and normal electric field at the interface. These equations are then easily solved using moment methods.⁶

II. THEORY

As a canonical problem for MFI, we choose a geometry consisting of two infinite, perfectly conducting, parallel plates separated by a distance a , as shown in Fig. 1. Parallel to the y

Fig. 1. Geometry for two-dimensional problem.

axis, there is a dielectric interface which is slanted at an angle α relative to the conducting plates. This interface is described by the equation

$$z_s = \beta x - b, \quad 0 < x < a, \quad (1)$$

where $\beta = \cot \alpha = 2b/a$ ($2b$ is the extent of the interface along the plates as shown in Fig. 1). To the left of the interface ($z < z_s$) is Region 1 with permittivity ϵ_1 and to the right of the interface ($z > z_s$) is Region 2 with permittivity ϵ_2 . The problem is time-independent (electrostatic) and independent of the y coordinate. The plate at $x = a$ is assumed to be at a potential V relative to the lower plate.

The electric scalar potential ϕ must satisfy Poisson's equation

$$\nabla^2 \phi = -\rho/\epsilon \quad (2)$$

subject to the boundary conditions

$$\begin{aligned} \phi &= 0, & x &= 0, \\ \phi &= V, & x &= a, \\ \phi_1 &= \phi_2, & \text{on the interface} \end{aligned} \quad (3)$$

$$\epsilon_1 \frac{\partial \phi_1}{\partial \eta} - \epsilon_2 \frac{\partial \phi_2}{\partial \eta} = \rho_s, \quad \text{on the interface}.$$

ρ_s and ρ are the surface charge density on the interface and the charge density between the plates, respectively, and η is the

normal direction to the interface (see Fig. 1). The subscripts 1 and 2, when used, refer to those quantities in Region 1 or 2, respectively. When this subscript is omitted, the reference is to the particular quantity in either region.

In order to obtain an integral equation for this problem, one must first define an appropriate Green's function, which in this case is defined by

$$\nabla^2 g = -\delta(x - x')\delta(z - z') \quad (4a)$$

with

$$g = 0, \quad x = 0 \text{ and } x = a, \quad (4b)$$

$$g, \partial g / \partial z \rightarrow 0, \quad z \rightarrow \pm\infty.$$

Now using Green's theorem and the properties of the Green's function, one can obtain the following expression for the potential

$$\begin{aligned} \phi_i(\bar{x}) = & \frac{1}{\epsilon_i} \int_{V_i} g(\bar{x}, \bar{x}') \rho(\bar{x}') dv' \\ & + \oint_{S_i} [g(\bar{x}, \bar{x}') \nabla' \phi_i(\bar{x}') - \phi_i(\bar{x}') \nabla' g(\bar{x}, \bar{x}')] \cdot \hat{n}_i ds' \end{aligned} \quad (5)$$

where $i = 1$ or 2 , V_i , S_i , and $\hat{n}_i$ are the volume, closed surface, and the outward normal unit vector for Region 1 or 2, respectively, and the vector $\bar{x}$ represents (x, z) . By taking the appropriate derivative of (5), one obtains the electric field normal to the interface, i.e.,

$$\begin{aligned}
\epsilon_i \frac{\partial}{\partial \eta} \phi_i(\bar{x}) &= \frac{\partial}{\partial \eta} \int_{V_i} g(\bar{x}, \bar{x}') \rho(\bar{x}') dv' \\
&+ \epsilon_i \frac{\partial}{\partial \eta} \oint_{S_i} [g(\bar{x}, \bar{x}') \nabla' \phi_i(\bar{x}') - \phi_i(\bar{x}') \nabla' g(\bar{x}, \bar{x}')] \cdot \hat{n}_i ds'
\end{aligned} \tag{6}$$

Note that because of the choice of boundary conditions on g , the only surviving portions of the surface integrals in (5) and (6) are along the interface and the $\phi \nabla' g$ term along the upper conducting plate.

The final step in obtaining the integral equations for ϕ and $\partial \phi_1 / \partial \eta$ at the interface is to use the interface boundary conditions on ϕ from (3) to eliminate ϕ_2 and $\partial \phi_2 / \partial \eta$ from (5) and (6) and then force these equations to be self-consistent as $\bar{x}$ approaches the interface from either side, i.e.,

$$\begin{aligned}
\phi(\bar{x}) &= \frac{1}{\epsilon_2} \int_{V_2} g(\bar{x}, \bar{x}') \rho(\bar{x}') dv' \\
&- \int_B \left\{ g(\bar{x}, \bar{x}') \left[\frac{\epsilon_1}{\epsilon_2} \frac{\partial \phi_1}{\partial \eta'}(\bar{x}') - \frac{1}{\epsilon_2} \rho_s(\bar{x}') \right] \right. \\
&\left. - \phi(\bar{x}') \frac{\partial g}{\partial \eta'}(\bar{x}, \bar{x}') \right\} dl' - V C_2(\bar{x}) \quad ,
\end{aligned} \tag{7}$$

as $\bar{x}$ approaches the interface from Region 2, where B is the interface boundary and

$$\begin{aligned}
\varepsilon_1 \frac{\partial \phi_1}{\partial \eta}(\bar{x}) &= \frac{\partial}{\partial \eta} \int_{V_1} g(\bar{x}, \bar{x}') \rho(\bar{x}') dv' \\
&+ \varepsilon_1 \frac{\partial}{\partial \eta} \int_B [g(\bar{x}, \bar{x}') \frac{\partial \phi_1}{\partial \eta'}(\bar{x}') \\
&- \phi(\bar{x}') \frac{\partial g}{\partial \eta'}(\bar{x}, \bar{x}')] dl' - \varepsilon_1 v \frac{\partial C_1}{\partial \eta}(\bar{x}), \quad (8)
\end{aligned}$$

as $\bar{x}$ approaches the interface from Region 1. The functions C_1 and C_2 are the surviving integrals along the upper plate from (5) and (6), respectively, and are given by

$$C_1(\bar{x}) = \int_{-\infty}^b \frac{\partial g}{\partial x'}(\bar{x}, \bar{x}') \Big|_{x'=a} dz' \quad (9)$$

and

$$C_2(\bar{x}) = \int_b^{\infty} \frac{\partial g}{\partial x'}(\bar{x}, \bar{x}') \Big|_{x'=a} dz'.$$

Now it remains to determine the Green's function which satisfies (3). This is easily done using standard techniques: first, expand g in a Fourier sine series in x , substitute into (4a), then use the orthogonality of the Fourier expansion functions to obtain a one-dimensional Green's function equation in z . This equation is solved by standard methods,⁷ i.e., forcing continuity of g and the jump condition on dg/dz at $z = z'$. The resulting expression for the Green's function is

$$g(\bar{x}, \bar{x}') = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{e^{-n\gamma|z-z'|}}{n} \sin n\gamma x \sin n\gamma x' \quad (10)$$

where $\gamma = \pi/a$. A closed form expression can be obtained for g (see 10.204 in Ref. 8),

$$g(\bar{x}, \bar{x}') = \frac{1}{4\pi} \ln \frac{\cosh \gamma|z - z'| - \cos \gamma(x + x')}{\cosh \gamma|z - z'| - \cos \gamma|x - x'|} \quad (11)$$

Both expressions for g will be useful in what follows.

III. NUMERICAL IMPLEMENTATION

An effective technique for the numerical solution of integral equations is the method of moments⁶ which converts an integral equation into a matrix equation. Consider the operator equation

$$L\bar{u} = \bar{f} \quad , \quad (12)$$

where L is a linear operator, $\bar{f}$ is a known vector, and $\bar{u}$ is an unknown vector for which a solution is desired. Using the method of moments, one approximates $\bar{u}$ by a finite linear combination of expansion vectors $\bar{u}_i$. Thus, let

$$\bar{u} = \sum_{i=1}^N a_i \bar{u}_i \quad (13)$$

Now take the inner product of (12) with N testing vectors $\bar{w}_j$. If (13) is substituted into this result, and L is linear, the following matrix equation is obtained:

$$\sum_{i=1}^N \langle \bar{w}_j, L\bar{u}_i \rangle a_i = \langle \bar{w}_j, \bar{f} \rangle, \quad j = 1, 2, 3, \dots, N. \quad (14)$$

Although this technique allows considerable flexibility in the choice of expansion and testing functions, in this problem the simple case of pulse expansion and delta testing will be used, i.e., expand

$$\phi(\bar{x}_s) = \sum_{i=1}^N a_i p_i(x_s) \quad (15a)$$

and

$$\frac{\partial \phi_1}{\partial \eta}(\bar{x}_s) = \sum_{i=1}^N b_i p_i(x_s) \quad (15b)$$

where $\bar{x}_s$ is a point on the boundary defined by (1) and

$$p_i(x) = \begin{cases} 1, & x_i > x > x_{i+1} \\ 0, & \text{otherwise} \end{cases}, \quad (16)$$

$$x_i = (i - 1)\Delta x, \quad \Delta x = a/N.$$

Now define the inner product and testing functions to be

$$\langle \bar{u}, \bar{v} \rangle = \int_B u(x) v(x) dl \quad (17)$$

$$\bar{w}_j(x) = \delta(x - x_j) \quad (18)$$

respectively, where

$$x_j = (j - 1/2)\Delta x. \quad (19)$$

It is useful at this point to make some limiting assumptions which will not be restrictive to the MFI problem. First, assume that Region 1 is vacuum with permittivity ϵ_0 and the dielectric constant in Region 2 is κ . Further, assume that there is no charge density ($\rho = 0$) in Region 2. Region 1 is divided into L subvolumes ΔV_ℓ , and within each of these subvolumes the charge density is assumed to be a constant value ρ_ℓ . Finally, we assume that the surface charge density on the interface can be approximated by

$$\frac{\rho_s(\bar{x}_s)}{\epsilon_0} = \sum_{i=1}^N r_i p_i(x_s) \quad (20)$$

If (14-20) are now applied, (7) and (8) become

$$\begin{aligned} \sum_{i=1}^N Q_{ji} b_i + \sum_{i=1}^N R_{ji} a_i = \\ -V C_2(\bar{x}_j) + \sum_{i=1}^N Q_{ji} r_i, \quad j = 1, 2, 3, \dots, N, \end{aligned} \quad (21)$$

and

$$\begin{aligned} \sum_{i=1}^N S_{ji} b_i + \sum_{i=1}^N T_{ji} a_j = \\ V \frac{\partial C_1}{\partial \eta}(\bar{x}_j) + \sum_{\ell=1}^L E_{j\ell} \rho_\ell, \quad j = 1, 2, 3, \dots, N, \end{aligned} \quad (22)$$

where

$$Q_{ji} = \frac{1}{\kappa} \csc \alpha \int_{x_i}^{x_{i+1}} g(\bar{x}_j, \bar{x}') dx' , \quad (23a)$$

$$R_{ji} = -\csc \alpha \int_{x_i}^{x_{i+1}} \frac{\partial g}{\partial \eta'}(\bar{x}_j, \bar{x}') dx' + \delta_{ij} , \quad (23b)$$

$$S_{ji} = \csc \alpha \frac{\partial}{\partial \eta} \int_{x_i}^{x_{i+1}} g(\bar{x}_j, \bar{x}') dx' - \delta_{ij} , \quad (23c)$$

$$T_{ji} = -\csc \alpha \frac{\partial}{\partial \eta} \int_{x_i}^{x_{i+1}} \frac{\partial g}{\partial \eta'}(\bar{x}_j, \bar{x}') dx' , \quad (23d)$$

$$E_{j\ell} = -\frac{1}{\epsilon_0} \frac{\partial}{\partial \eta} \int_{\Delta V_\ell} g(\bar{x}_j, \bar{x}') dv' , \quad (23e)$$

and the vector $\bar{x}_j$ represents the point on the interface $[x_j, z(x_j)]$, where $z(x)$ is defined by (1). Note that the expressions for these matrices rely on the fact that z' is a function of x' on the interface and that $dl' = \csc \alpha dx'$. Analytic, closed form expressions for R , S , T , C_2 , and $\partial C_1 / \partial \eta$ can be found (see appendix for details) and are given by

$$\begin{aligned}
R_{ji} = & \frac{s(z_j - z')}{2\pi} \left[\tan^{-1} \left\{ \frac{\sin \gamma(x_j + x')}{e^{\gamma|z_j - z'|} - \cos \gamma(x_j + x')} \right\} \right. \\
& + \left. \tan^{-1} \left\{ \frac{\sin \gamma(x_j - x')}{e^{\gamma|z_j - z'|} - \cos \gamma(x_j - x')} \right\} \right]_{x'=x_i}^{x_{i+1}} + \delta_{ij} [1 - x_j/a] , \\
\end{aligned}
\tag{24a}$$

$$\begin{aligned}
\varepsilon_{ji} = & \frac{1}{2\pi} \left[\tan^{-1} \left\{ \frac{\sin \gamma|x_j - x'|}{e^{\gamma|z_j - z'|} - \cos \gamma|x_j - x'|} \right\} \right. \\
& - s(z_j - z') \cos 2\alpha \tan^{-1} \left\{ \frac{\sin \gamma(x_j + x')}{e^{\gamma|z_j - z'|} - \cos \gamma(x_j + x')} \right\} \\
& + \left. \frac{\sin 2\alpha}{2} \left\{ \gamma|z_j - z'| - \ln[\cosh \gamma|z_j - z'| - \cos \gamma(x_j + x')] \right\} \right]_{x'=x_i}^{x_{i+1}} \\
& + \delta_{ij} [(x_j/a) \cos 2\alpha - \cos^2 \alpha] , \\
\end{aligned}
\tag{24b}$$

$$T_{ji} = \frac{s(z_j - z')}{4a}$$

$$\left[\frac{[e^{-\gamma|z_j - z'|} - \cos \gamma(x_j + x')] \cos \alpha - s(z_j - z') \sin \gamma(x_j + x') \sin \alpha}{\cosh \gamma|z_j - z'| - \cos \gamma(x_j + x')} \right. \\ \left. + \frac{[e^{-\gamma|z_j - z'|} - \cos \gamma|x_j - x'|] \cos \alpha - \sin \gamma|x_j - x'| \sin \alpha}{\cosh \gamma|z_j - z'| - \cos \gamma|x_j - x'|} \right]_{x'=x_i}^{x_{i+1}}$$

$$+ \delta_{ij} (\cos \alpha)/a, \quad (24c)$$

$$C_2(\bar{x}) = -\frac{1}{\pi} \tan^{-1} \left[\frac{\sin \gamma x}{e^{\gamma|b-z|} + \cos \gamma x} \right] \quad (25a)$$

$$\frac{\partial C_1}{\partial \eta}(\bar{x}) = \frac{1}{2a} \frac{\cos(\alpha - \gamma x) + \cos \alpha e^{\gamma|b-z|}}{\cosh \gamma(b-z) + \cos \gamma x} \quad (25b)$$

where $s(w) = (w/|w|)$ is the sign of w . There is no convenient closed form for Q or E , so they have been computed numerically using 4 point Gaussian quadrature for Q and rectangular integration for E .

Special care must be taken in the computation of Q , R , S , and T , when i equals j . In this case, the integrands in (23) are

singular (but necessarily are integrable) and consequently these terms must be considered separately. The details on the evaluation of these self-terms can be found in the appendix. Note that the effect of these singularities result in the δ_{ij} terms in (24).

Using standard matrix techniques, the coupled matrix equations (21) and (22) can be solved for ϕ and $\partial\phi_1/\partial\eta$ along the interface (i.e., a_i and b_i , $i = 1, 2, 3, \dots, N$). Now the potential and electric field can be determined everywhere by quadrature using (7) and the gradient of (7). Of particular interest to our application is the potential at the point $\bar{x}_k$ in Region 1, which, in matrix form is given by

$$\phi_1(\bar{x}_k) = \sum_{i=1}^N Q_{ki} b_i + \sum_{i=1}^N R'_{ki} a_i + \sum_{\ell=1}^L F_{k\ell} \rho_\ell - V C_1(\bar{x}_k) , \quad (26)$$

where

$$R'_{ki} = \Gamma(\bar{x}_k, \bar{x}_{i+1}) - \Gamma(\bar{x}_k, \bar{x}_i) + p_i(x_0)(1 - x_k/a) , \quad (27)$$

$$\Gamma(\bar{x}, \bar{x}') = \frac{s(z-z')}{2\pi} \left\{ \tan^{-1} \left[\frac{\sin \gamma(x+x')}{e^{\gamma|z-z'|} - \cos \gamma(x+x')} \right] \right. \\ \left. + \tan^{-1} \left[\frac{\sin \gamma(x-x')}{e^{\gamma|z-z'|} - \cos \gamma(x-x')} \right] \right\} , \quad (28)$$

$$F_{k\ell} = \frac{1}{\epsilon_0} \int_{\Delta V_\ell} g(\bar{x}, \bar{x}') dv' \quad (29)$$

$$C_1(\bar{x}) = -x/a - C_2(\bar{x}) \quad , \quad (30)$$

and $\bar{x}_0 = (x_0, z_k)$ where $x_0 = (z_k + b)/\beta$. The vector $\bar{x}_0$ is the point along the interface plane defined by $z_0 = z_k$. Note that (28) is discontinuous at $x' = x_0$ and consequently the extra term in (27) is needed when the range of integration includes this discontinuity. The integrand in $F_{k\ell}$ is singular when $\bar{x}_k$ is in ΔV_ℓ . As before, this self-term must be handled separately (as shown in the appendix).

IV. SAMPLE NUMERICAL RESULTS

In all the accompanying results, the same geometry has been used with various charge density distributions to help illustrate convergence properties of the method and to compare the moment method solution to a finite difference solution using the Alternating Direction Implicit (ADI) technique.^{4,5} In all cases shown, the geometrical constants used are: $a = 1.0$, $b = .25$, and $\kappa = 2.5$. In the ADI solution, Neumann boundary conditions are enforced at $z/a = \pm 1.25$. Unless otherwise specified, the number of grid points along the interface (N) will be 20.

In Fig. 2, the integral equation or moment method solution is shown to converge as N increases. Plots of the electric scalar potential and the electric field evaluated on the interface are shown for $N = 10, 20$, and 40 for two different charge density distributions. The first and simplest case (Fig. 2a) is charge-free, while the second example (Fig. 2b) has a unit surface charge on the interface between the two regions (i.e., $\rho_s/\epsilon_0 = +1$). With the exception of the normal electric field near the plates, the solution is seen to converge very rapidly.

Fig. 2a. Convergence of the moment method solution for the electric potential and field on the interface for $N = 10, 20, \text{ and } 40$ for a charge-free region.

Fig. 2b. Convergence of the moment method solution for the electric potential and field on the interface for $N = 10, 20$, and 40 for a unit surface charge on the interface.

The poorer convergence near the plates is not surprising since the electric field on the interface is known to be rapidly varying (possibly singular) near the plates.⁹ This can be demonstrated by considering a polar coordinate system (r, θ) centered at the triple-point where the plate and both dielectric media meet (this problem has two such points). The r and θ components of the electric field can then be expanded in power series in r with θ -dependent coefficients. By applying $\nabla \cdot \vec{E} = \nabla \times \vec{E} = 0$, then solving the resulting ordinary differential equation in θ for the lowest power of r subject to the appropriate boundary conditions in θ , we can show that $\vec{E}$ varies as r^τ for small r , where τ is given by

$$\tan[\lambda_2(1+\tau)] + \kappa \tan[\lambda_1(1+\tau)] = 0 \quad . \quad (31)$$

In (31), λ_1 and λ_2 are the wedge angles of Regions 1 and 2 at the triple-point, respectively. A more detailed description of this derivation for a slightly more complicated problem can be found in Ref. 10. Figure 3 shows the solution of (31) for several values of κ for the case $\lambda_1 + \lambda_2 = \pi$. For acute values of λ_2 , the homogeneous field goes to zero at the triple-point, but to a very low fractional power, consistent with Fig. 2a at $x/a = 0$. For obtuse values of λ_2 , the homogeneous field is singular at the triple-point as indicated by Fig. 2a at $x/a = 1$.

In Fig. 4, the moment method and the ADI method solutions are compared for a point charge in Region 1 with magnitude $\rho/\epsilon_0 = \Delta x \Delta z \delta(\bar{x})$ where $x/a = 0.5$, and $z/b = -0.8$. The two solutions are in agreement for the potential and the normal field on the interface,

Fig. 3. Asymptotic dependence of the electric field ($E \propto r^\tau$) on the distance from the triple-point (r) as a function of wedge angle (λ_2) for several different dielectric constants (κ).

Fig. 4a. Comparison of integral equation (moment method) and ADI solver solutions for a point charge in Region 1 showing the electric potential and field on the interface.

Fig. 4b. Comparison of integral equation (solid) and ADI (dashed) solutions for a point charge in Region 1 showing equipotentials over the entire volume. The spacing between the contours, $\Delta\phi$, is given by $\Delta\phi = 0.1$ V.

as shown in Fig. 4a. In Fig. 4b, a plot of equipotential contours is shown. There are only slight differences between the solutions in the vicinity of the point charge. This difference is due to the different way in which a point charge is treated by the two techniques.

For the results shown in Fig. 5, a charge density distribution of $\rho/\epsilon_0 = f(x,z)$ was used, where

$$f(x,z) = \max[0, 1 - |z - (\beta x - 2b)|/b]$$

This represents a triangular charge density distribution whose peak is located a distance b from the interface and whose base is $2b$, as shown in Fig. 6. Again, the solutions on the interface are in agreement, as shown in Fig. 5a. In Fig. 5b, one of the main differences in the two codes becomes apparent. The ADI method enforces Neumann boundary conditions at the left and right boundaries, which is only a good approximation away from the interface or any charge. The moment method does not have this problem since the infinite integral which arises in the problem formulation can be evaluated. In the example of Fig. 4b, the boundaries were far enough from the interface and any charge so that the Neumann boundary conditions are fairly accurate and hence the solutions agree. In Fig. 5b, however, the presence of the large amount of charge near the left boundary causes a significant non-zero normal derivative at that boundary. Consequently, the ADI method, unlike the moment method, needs a larger grid to provide a buffer zone to separate the boundaries from the interface and any charge. (Although this buffer zone is necessary for

Fig. 5a. Comparison of integral equation (moment method) and ADI solver solutions for a triangular charge density distribution in Region 1 showing the electric potential and field on the interface.

Fig. 5b. Comparison of integral equation (solid) and ADI (dashed) solutions for a triangular charge density distribution in Region 1 showing equipotentials over the entire volume. The spacing between the contours, $\Delta\phi$, is given by $\Delta\phi = 2.0$ V.

Fig. 6. Triangular charge density distribution $[f(x, z)]$ as a function of $z - z_0(x)$, where $z_0(x) = \beta x - 2b$.

the accuracy of the ADI solution, the added computational cost can be minimized using nonuniform gridding techniques.)

V. CONCLUSIONS

Moment methods have been used to solve the problem of an arbitrarily oriented dielectric interface between two perfectly conducting parallel plates. This has involved the derivation of a set of coupled integral equations using Green's theorem and their subsequent numerical solution. Results have been obtained for several different examples of charge density distributions, both on the interface and on the vacuum side of the interface. The solutions have been shown to be in good agreement with those derived from the ADI method.

Although this method was developed as a check of the ADI potential solver in a 2-D PIC code, it soon became apparent that a hybrid PIC code in which the ADI solver is replaced by the moment method solver could quite possibly have several advantages. For example, in the ADI solver, the interface must pass diagonally through consecutive points on the grid. Because of limitations on the aspect ratio of a grid cell, some practical limits are placed on the value of α . The moment method places no such restriction on α . Preliminary comparisons seem to indicate that the moment solution for the normal field near the triple-point is more accurate than the ADI solution. Another potential advantage arises because the ADI solver must compute potentials over a large 2-D grid, regardless of whether or not there is any charge at that location. In addition, many of these grid points are included only to provide a buffer so that the Neumann boundary

conditions applied are in fact accurate. On the other hand, the moment solution need only compute potentials where there is charge and has no buffer requirements. One final possible advantage is that for a given value α , a matrix inversion is required only once; after that, only matrix multiplication is required.

Potential disadvantages of the method which need to be considered are the possibility of larger storage and time requirements. Storing the inverse of the matrix saves on time requirements, but uses up memory space. By far, the largest user of storage will be matrices which relate points on the interface (N) to points on a grid over Region 1 ($K \times N$). Computation time will be reduced by storing these matrices rather than recomputing them at each time step in the PIC code; however, each of these matrices will require KN^2 words of memory. This requirement can be substantially reduced, however, by noting that the arguments of the functions depend only on the sum or difference of their x coordinates, and only on the difference of their z coordinates. Using this property of the matrices allows a reduction in the storage required to approximately $3KN$ for each matrix. A fair comparison of the relative speeds of the two methods has not yet been performed and will require the implementation of the storage scheme outlined above.

The future direction of this work will include the development of a hybrid code, which hopefully will provide significant improvements in speed, accuracy, and/or generality. Indeed, the demonstration of such improvements will be an important part of our effort. If this hybrid code in fact has some advantages, it

will be available to treat the specific problem of MFI as well as other problems which may in the future arise involving dielectric interfaces in similar geometries.

VI. ACKNOWLEDGMENTS

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APPENDIX

This appendix details the derivation of (24) and (25) from (9) and (23). Also included is the evaluation of (29) for the self-term, i.e., when $k = \ell$. In all cases, the integrands are singular and require very careful consideration of the limiting process.

First, we consider the derivation of (24). Complete details will be shown for (24a) and (24c); (24b) can be obtained using essentially the same techniques. We start by using (10) and recognizing that

$$\partial g / \partial \eta' = (\partial g / \partial x')(\partial x' / \partial \eta') + (\partial g / \partial z')(\partial z' / \partial \eta') \quad (A1)$$

and that

$$\partial x' / \partial \eta' = -\cos \alpha, \quad \partial z' / \partial \eta' = \sin \alpha \quad (A2)$$

to obtain

$$\begin{aligned} \partial g / \partial \eta' = & \\ \sum_{n=1}^{\infty} \frac{e^{-n\gamma|z-z'|}}{a} & \sin n\gamma x [s(z-z') \sin \alpha \sin n\gamma x' - \cos \alpha \cos n\gamma x'] \end{aligned} \quad (A3)$$

This expression is now integrated over a section of the interface defined by $X_1 < x' < X_2$, using the relationships that $dl' = \csc \alpha dx'$ and $z' = \beta x' - b$, to give

$$I_1 = \frac{\csc \alpha}{a} \sum_{n=1}^{\infty} e^{-s(z-z')n\gamma(z+b)} \sin n\gamma x \int_{X_1}^{X_2} e^{s(z-z')n\beta\gamma x'} [s(z-z') \sin \alpha \sin n\gamma x' - \cos \alpha \cos n\gamma x'] dx' \quad (A4)$$

This expression can then be integrated (see 575.1 and 576.1 of Ref. 11) to give

$$I_1 = \frac{\csc \alpha}{a} \sum_{n=1}^{\infty} \frac{1}{n} e^{-s(z-z')n\gamma(z+b)} \sin n\gamma x \left[e^{s(z-z')n\beta\gamma x'} \left\{ s(z-z') \sin \alpha [s(z-z')\beta \sin n\gamma x' - \cos n\gamma x'] - \cos \alpha [s(z-z')\beta \cos n\gamma x' + \sin n\gamma x'] \right\} \right]_{x'=X_1}^{X_2} \quad (A5)$$

which after some algebraic manipulation (and recognizing that $\cos \alpha = \beta \sin \alpha$) becomes

$$I_1 = \frac{-s(z-z')}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\gamma|z-z'|} \left[\sin n\gamma(x+x') + \sin n\gamma(x-x') \right]_{x'=X_1}^{X_2} \quad (A6)$$

This infinite sum can be expressed in closed form (Ref. 8, 10.202) as

$$I_1 = -\frac{s(z-z')}{2\pi} \left\{ \tan^{-1} \left[\frac{\sin \gamma(x+x')}{e^{\gamma|z-z'|} - \cos \gamma(x+x')} \right] + \tan^{-1} \left[\frac{\sin \gamma(x-x')}{e^{\gamma|z-z'|} - \cos \gamma(x-x')} \right] \right\} \Bigg|_{x'=x_1}^{x_2} \quad (A7)$$

To evaluate (23d) we now need to differentiate (A6) with respect to the unprimed normal component. We will denote this term by I_2 which by differentiation becomes

$$I_2 = \frac{s(z-z')}{2a} \sum_{n=1}^{\infty} e^{-n\gamma|z-z'|} \left[s(z-z') \sin \alpha \left\{ \sin n\gamma(x+x') + \sin n\gamma(x-x') \right\} + \cos \alpha \left\{ \cos n\gamma(x+x') + \cos n\gamma(x-x') \right\} \right] \Bigg|_{x'=x_1}^{x_2} \quad (A8)$$

This expression can be reduced to closed form using (10.201) and (10.203) of Ref. 8 to yield (24c).

The expressions in (A7) and (A8) have been obtained without careful consideration of the discontinuities of the integrands at $z = z'$ or of the limiting process as the observation point ($\bar{x}$) approaches the interface. This approach is sufficient for "non-self" terms and combining (A7) and (23b) produces (24a) for $i \neq j$. However, to properly treat the $i = j$ terms, it is necessary to deal with both the integrand discontinuities and the limit.

To treat the self-term, we need to take the limit as the unprimed coordinate approaches the point $\bar{x}_0$ on the interface. To do this, it is convenient to express $\bar{x}$ in terms of η by

$$z = z_0 + \eta \sin \alpha, \quad x = x_0 - \eta \cos \alpha. \quad (A9)$$

Now, to let the observation point $\bar{x}$ approach the boundary from Region 1 or Region 2, we simply let η approach zero from below or above, respectively. Since the Green's function kernel is a function of $|z - z'|$, the integral must be split into two parts at $z = z'$. Thus, for the self-term, we need to integrate x' from X_1 to $x_\ell - \epsilon$, and then from $x_\ell + \epsilon$ to X_2 in the limit as ϵ approaches zero where x_ℓ is the value of x along the interface where $z = z'$, i.e.,

$$x_\ell = (z + b)/\beta = (z_0 + b + \eta \sin \alpha)/\beta. \quad (A10)$$

Note that since the kernel is singular, we need to also examine the contribution (if any) from the integral over $x_\ell \pm \epsilon$. Consequently, the self-term expression of (24a) will include (A7), plus contributions from the intermediate integration endpoints $x_\ell \pm \epsilon$, plus any contributions from the infinitesimal integration over the singularity. It is important that we take all limits in a consistent fashion, i.e., we will let $\epsilon \rightarrow 0$ before we let $\eta \rightarrow 0$ in all cases.

First consider the intermediate endpoint contributions for the upper and lower halves of the integral. First, we substitute (A9) into (A6) and evaluate at $x' = x_\ell \pm \epsilon$ rather than X_1 and X_2 to obtain

$$I_1' = \frac{-s(z-z')}{2\pi} \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\gamma|z_0 + \eta \sin \alpha - z'|} \left\{ \sin n\gamma(x_0 - \eta \cos \alpha + x') \right. \\ \left. + \sin n\gamma(x_0 - \eta \cos \alpha - x') \right\} \Big|_{x'=x_0+\epsilon}^{x_0-\epsilon} \quad (A11)$$

If we now let $\epsilon \rightarrow 0$, (A11) becomes

$$I_1' = -\frac{1}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left\{ \sin n\gamma \left[2x_0 + \frac{\sin \alpha}{\beta} \eta (1-\beta^2) \right] - \sin n\gamma \left[\frac{\sin \alpha}{\beta} \eta (1+\beta^2) \right] \right\} \quad (A12)$$

Using (10.101) in Ref. 8 and extending it to $0 > x > -2\pi$, we obtain

$$\sum_{n=1}^{\infty} \frac{\sin nx}{n} = 2\pi u(x) - (\pi+x) \quad , \quad -2\pi < x < 2\pi \quad (A13)$$

where $u(x)$ is the unit step function. Now we combine (A13) with (A12) and perform some algebraic simplification to obtain

$$I_1' = u(\eta) - 1 + (x - \eta \cos \alpha)/a \quad (A14)$$

which represents the intermediate endpoint contributions to (24a). To obtain the similar contributions to (24c), we simply differentiate (A14) with respect to η , i.e.,

$$I_2' = \delta(\eta) - (\cos \alpha)/a \quad , \quad (A15)$$

Finally, we need to consider the infinitesimal portion of the integral. Since the range of the integration is infinitesimal,

only the singularities of the kernel will contribute. These singularities are completely contained in the free space Green's function and consequently it is sufficient to integrate only that portion of the kernel. Consider the free space kernel g_0 given by⁷

$$g_0(\bar{x}, \bar{x}') = 1/(4\pi) \ln[(\eta - \eta')^2 + (\ell - \ell')^2] . \quad (A16)$$

We will assume for simplicity that the interface is at $\eta = 0$ and that the observation point will approach the interface normally at $\ell = 0$. Consequently, the derivative of g_0 with respect to η' evaluated at the interface ($\eta' = 0$) is given by

$$\partial g_0 / \partial \eta' = -1/(2\pi) \eta / (\eta^2 + \ell^2) . \quad (A17)$$

Next we integrate (A17) over ℓ' from $-\epsilon$ to ϵ to obtain

$$I_1'' = (1/\pi) \tan^{-1} (\epsilon/\eta) = (1/\pi) \cot^{-1} (\eta/\epsilon) \quad (A18)$$

Now differentiate (A18) with respect to η to obtain

$$I_2'' = (-1/\pi) \epsilon / (\epsilon^2 + \eta^2) . \quad (A19)$$

Finally, as we let ϵ approach zero, (A18) and (A19) become¹²

$$I_1'' = 0 \quad (A20)$$

and

$$I_2'' = -\delta(\eta) . \quad (A21)$$

By combining (23b), (A7), (A14) and (A20), we finally produce (24a). Similarly, (23d), the closed form of (A8), (A15) and (A21) combine to give (24c). Note that the $\delta(\eta)$ terms in (A15) and (A21) cancel

one another (as they must since the electric field is certainly finite at the interface). These terms are the result of the way the integral was broken up, and their presence demonstrates the necessity of careful application of the limiting process.

As mentioned earlier, there is no convenient closed form evaluation of (23a), and it is simpler to use numerical quadrature using (11) for this evaluation. However, this will obviously not work for the self-term since (11) is singular at $\bar{x} = \bar{x}'$. The Green's function (11) can be written as the sum of a singular and nonsingular term as

$$g(x, x') = (1/4\pi) \ln[\cosh \gamma|z-z'| - \cos \gamma(x+x')] + g_s(y) \quad (A22)$$

where

$$g_s(y) = (-1/4\pi) \ln(\cosh \beta\gamma y - \cos \gamma y) \quad , \quad (A23)$$

$$y = |x - x'| \quad , \quad \beta y = |z - z'| \quad .$$

For $(\beta + 1)\gamma y \ll 1$, we can approximate (A23) with Taylor series expansions as

$$g_s(y) \approx \frac{1}{4\pi} \ln \left\{ \left[1 + \frac{(\gamma\beta y)^2}{2} + \frac{(\gamma\beta y)^4}{24} \right] - \left[1 - \frac{(\gamma y)^2}{2} + \frac{(\gamma y)^4}{24} \right] \right\} \quad (A24)$$

which after some manipulation becomes

$$g_s(y) \approx (-1/4\pi) [\ln(a_1 y^2) + \ln(1 + a_2 y^2)] \quad (A25)$$

where

$$a_1 = \gamma^2(\beta^2 + 1)/2 \quad , \quad a_2 = \gamma^2(\beta^2 - 1)/12 \quad . \quad (A26)$$

This can be integrated (see, for example, Ref. 11) to yield

$$\int_0^y g_s(y') dy' = (y/4\pi) \{ 4 - \ln[a_1 y^2 (1 + a_2 y^2)] - f(a_2) \} \quad (A27)$$

where

$$f(a_2) = \frac{1}{a_3} \begin{cases} \ln(1 + a_3 y) - \ln(1 - a_3 y) & , \quad a_2 > 0 \\ 2 \tan^{-1}(a_3 y) & , \quad a_2 < 0 \end{cases} \quad (A28)$$

and $a_3 = |a_2|^{1/2}$.

Next, we consider the derivation of (25). The derivative of the Green's function (10) is

$$\frac{\partial g}{\partial x'} = \sum_{n=1}^{\infty} e^{-n\gamma|z-z'|} \sin n\gamma x \cos n\gamma x' \quad (A29)$$

Evaluating this expression at $x' = a$ and then integrating over z' , first from $-\infty$ to b , then from b to $+\infty$ (separating the integral at $z = z'$ because of the $|z - z'|$ dependence), we obtain

$$C_1(\bar{x}) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin n\gamma x [2 - e^{n\gamma(b-z)}] \quad , \quad (A30)$$

and

$$C_2(\bar{x}) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin n\gamma x [2 u(z-b) + e^{-n\gamma|b-z|}] \quad . \quad (A31)$$

In the derivation of (A30), we have made use of the fact that $z < b$ always in Region 1. Using (10.107) and (10.202) of Ref. 8 and the following identity

$$(-1)^n \sin n\gamma x = -\sin n\gamma(a-x) ,$$

(A30) and (A31) can be reduced to closed form as

$$C_1(\bar{x}) = \frac{1}{\pi} \tan^{-1} \left(\frac{\sin \gamma x}{e^{\gamma|b-z|} + \cos \gamma x} \right) - \frac{x}{a} , \quad (A32)$$

and

$$C_2(\bar{x}) = -\frac{1}{\pi} \tan^{-1} \left(\frac{\sin \gamma x}{e^{\gamma|b-z|} + \cos \gamma x} \right) - \frac{x}{a} u(z-b) . \quad (A33)$$

Note that (A33) becomes (25a) when $\bar{x}$ is on the interface (since $z < b$ on the interface). Using (A2) and the chain rule, (A32) can be differentiated with respect to η , and after some further algebraic simplification we obtain the expression given in (25b).

Finally, we consider the evaluation of (29). In all cases except the self-term, it is sufficient to use some type of two-dimensional numerical quadrature (a one-point rectangular rule was used for the results shown in this report). In the case of the self-term, we again make use of the fact that the free-space Green's function (A16) contains the entire singularity. Consequently, $g_h(\bar{x}, \bar{x}') = g(\bar{x}, \bar{x}') - g_0(\bar{x}, \bar{x}')$ is a slowly-varying function near $\bar{x} = \bar{x}'$ and can be adequately integrated using quadrature. Thus, we only need to consider the self-term integral of $g_0(\bar{x}, \bar{x}')$. Using a rectangular ΔV_ℓ with sides of length Δx and Δz , defining

$\bar{x}_\ell$ to be the geometric center of ΔV_ℓ and using (528.1), (623) and (623.1) of Ref. 11, we find that

$$\int_{\Delta V_\ell} g_o(\bar{x}, \bar{x}') dv' = (-1/4\pi) \{ \Delta x \Delta z [\ln(\Delta x^2 + \Delta z^2) - \ln 4 - 3] + \Delta x^2 \tan^{-1}(\Delta z/\Delta x) + \Delta z^2 \tan^{-1}(\Delta x/\Delta z) \} . \quad (A34)$$

This expression can now be added to the numerically determined integral of $g_h(\bar{x}, \bar{x}')$, resulting in the desired expression for (29).

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