Variational Solution of Integral Equations

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Abstract—A variational solution of the Fredholm integral equation of the first kind resulting from Laplace's equation with Dirichlet boundary conditions is discussed. Positive-definiteness of the integral operator is used to guarantee convergence. The square parallel plate capacitor is given as an example with several different types of trial functions. Special singular functions to handle known field behavior are shown to result in improved accuracy with reduced computing cost. The air–dielectric interface condition is related to a general Neumann-mixed boundary condition for which a variational method with a positive-definite integral operator is presented. Multiple boundary conditions are handled by mutually constraining separate variational expressions for each boundary condition. A T-shaped conductor on a dielectric slab, representative of quasi-static solutions of microstrip discontinuities, is presented as a three-dimensional example with multiple boundary conditions. Generally, it is shown how the finite-element method for the solution of partial differential equations may be extended to handle integral equation formulations.

I. Introduction

CONSIDER the real operator equation

$$Lu = f \tag{1}$$

where L is a self-adjoint positive-definite operator, i.e.,

$$\langle Lu,v\rangle = \langle u,Lv\rangle \tag{2}$$

and

$$\langle Lu,u\rangle \begin{cases} > 0, & u \neq 0 \\ = 0, & u = 0. \end{cases} \tag{3}$$

The pointed brackets denote an inner product of the functions located on alternate sides of the comma. The simplest form of inner product is the integration of the product over the domain of the problem.

In order to conveniently define the above-mentioned properties of L, the functions in (2) and (3) must satisfy homogeneous boundary conditions. However, this does not restrict the variational method to such a limited class of functions as any problem with inhomogeneous boundary conditions can be converted into one with homogeneous boundary conditions and additional source terms in f of (1) [2, p. 163].

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It is well known [3, pp. 74–95] that for a real self-adjoint and positive-definite operator, the functional

$$F = \langle Lu,u\rangle - 2\langle u,f\rangle \tag{4}$$

is minimized by the solution of (1). It is understood that all trial functions u must satisfy any requisite *principal* boundary conditions. It is also known that certain other boundary conditions will be satisfied without intervention. Hence, these latter ones are called *natural* boundary conditions.

In theory, (4) applies only to homogeneous boundary conditions. In practice, upon specification of the precise form of L, one can develop, from (4), the functional that must actually be used. This functional can then be made to accomodate inhomogeneous boundary conditions of both principal and natural types.

As an example of a partial differential equation consider the Poisson equation

$$-\nabla\cdot(\epsilon\nabla\phi) = \rho \tag{5}$$

in which the permittivity ϵ is a function of position. By the use of Green's identities, it is seen that the differential operator is both self-adjoint and positive-definite [1] when $\epsilon > 0$. From (4), with $u = \phi$, under a procedure described in [1] for inhomogeneous boundary conditions, we obtain

$$F = \iint_R [\epsilon(\nabla\phi)^2 - 2\phi\rho]\,dx\,dy - 2\int_C \phi h\,ds \tag{6}$$

for a 2-D region R with boundary $C + C'$. Trial functions must be restricted to satisfy the principal Dirichlet condition

$$\phi(s) = g(s), \qquad \text{on } C' \tag{7}$$

whereas the natural Neumann condition

$$\left.\frac{\partial\phi}{\partial n}\right|_s = h(s), \qquad \text{on } C \tag{8}$$

is satisfied automatically in the limit. (A more general functional for anisotropic media, is given in [5].) Efficient techniques for the minimization of such functionals is the subject of the finite-element method [6].

Note that the terms in (6) each correspond to electrostatic energy. If the functional is divided throughout by 2, the integral of the first term corresponds to the energy calculated entirely from electrostatic potential ϕ. The remainders of the second and the third integrals correspond to twice the energy calculated by using the real charge

$\rho(x,y)$ or the equivalent charge distribution $h(s)$ that can replace the inhomogeneous Neumann boundary condition. At the exact solution point, $F = F_{\min}$ which is the negative of the electrostatic energy of the field. At any other point, it turns out, from the nature of the operator, that the first integral increases relative to the other two so that $F > F_{\min}$. (The negative sign associated with $F_{\min}$ is irrelevant.) Thus the energy is minimized at the solution point.

Frequently, only the stationarity of a variational expression is employed. For example, if one is interested in the numerical value of F at the solution point (if, for instance, F is proportional to system energy, capacitance, etc.), then if ϕ is a "reasonable" estimate, F will be a "better" approximation due to the fact that F is stationary about the solution point. This is true whether F is minimal (because of L being positive-definite) or merely stationary (if L is not positive-definite). Little is said about the convergence of F or the field solution ϕ as the number of variational parameters is increased when the functional is only stationary.

But if L is positive-definite, then the Rayleigh–Ritz approximating procedure will not permit deterioration of the approximations of $F_{\min}$ and ϕ as extra terms are added. Convergence is guaranteed. Moreover, the method guarantees that the variational coefficients will be adjusted so as to produce the least value of F and the "best" (in the rms sense) possible solution of ϕ within the degree of approximation being used. We shall see, for example, that it is better to make a guess at the form of an unknown corner singularity rather than to ignore it altogether. Positive definiteness and the resulting guarantee of rapid convergence are of the most direct and significant consequence to computing costs.

The preceding description of the variational method has centered about the solution of partial differential equations. Indeed, the variational solution of field problems has been concerned exclusively with partial differential equations although integral equation formulations present some advantages, e.g., reduction of the dimensionality of problems. Therefore, one can expect storage demands and perhaps computing costs to be reduced. The obvious question then is the following: as the principles behind the variational method, summarized in (1)–(4), are general and not particular to partial differential equations, can we not devise a parallel development for integral equations?

II. Energy Functionals for Certain Integral Equations

The mathematical fact that the Laplacian operator is positive definite agrees with the physical fact that the energy $\langle -\nabla^2\phi,\phi\rangle = \iint (\nabla\phi)^2\, dx\, dy$ must be expended in order to establish the field. This energy is calculated from the electrostatic potential. It is physically obvious, since the field $\phi(x,y)$ may be described by a charge distribution over a conductor, that the associated integral operator should be positive-definite as well. After all, both mathematical formulations describe the model of the same physical system exactly.

In what follows, we shall not concern ourselves with particular Green's functions appropriate to particular problems. Such Green's functions are usually impossibly difficult to find analytically and, if available in certain cases, they are likely to be expressed as infinite summations or in other inconvenient forms. We shall replace conducting boundaries having prescribed potentials with charge distributions in free space having the same potentials. Furthermore, we shall replace any interface between permeable media by a distribution of polarization charge and consider that charge to exist in unbounded vacuum [7, pp. 183–185]. In so doing, we solve the equivalent problem of a charge distribution in free space knowing that we are at liberty to excise the region of original interest.

The integral form of the Poisson equation with a spatial charge distribution $\sigma(r)$ is

$$K\sigma(r) = \int \frac{\sigma(r')}{\epsilon_0} G(r \mid r')\, dr' = \phi(r) \tag{9}$$

in which the integration is performed over the entire free-space region. Equation (9) defines the integral operator K.

In two-dimensional space the free-space Green's function is [8, pp. 115–118]

$$G(r \mid r') = -\frac{1}{2\pi} \ln \mid r - r' \mid \tag{10}$$

and in three dimensions it is

$$G(r \mid r') = \frac{1}{4\pi \mid r - r' \mid} \tag{11}$$

where $\mid r - r' \mid$ is the distance between the observation and source points, r and r', respectively.

These Green's functions possess integrable singularities which must be carefully handled in numerical computation [9, pp. 410–430]. Appropriate techniques are described in Section III.

A. The Dirichlet Problem

The Dirichlet problem arises when we are given, as in Fig. 1,

$$\phi(s) = g(s) \tag{12}$$

and we are required to find $\sigma(s)$. For simplicity only, we shall consider such specified potentials and the resulting charges to exist only on surfaces. Thus (9) is written in the form

$$K\sigma(s) = \int_S \frac{\sigma(s')}{\epsilon_0} G(s \mid s')\, ds' = \phi(s). \tag{13}$$

An equation of the form of (13), with the unknown located within the integral operation, is known as a Fredholm integral equation of the first kind.

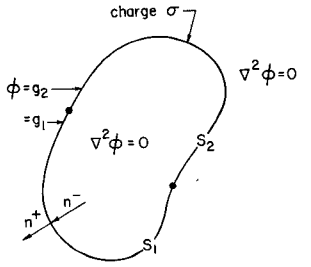

Fig. 1. Integral equation—problem configuration and conventions. Surface $S = S_1 U S_2$.

Any charge distribution will satisfy Laplace's equation at all points in the entire space *not* on the boundary S. However, only one charge distribution will satisfy a specific set of boundary conditions, i.e., the Fredholm equation of the first kind has a unique solution [10, pp. 277–315], [11, pp. 180–186]. On the surface itself, the Green's function is singular as is obvious from (10) and (11). In addition, the singularities in normal derivative of potential on alternate sides of the surface are known and are given by [8, pp. 115–123]

$$\frac{\partial \phi}{\partial n_-}(s) = \frac{\sigma(s)}{2\epsilon_0} + \int_S \frac{\sigma(s')}{\epsilon_0} \frac{\partial G}{\partial n}(s \mid s')\, ds' \tag{14a}$$

and

$$\frac{\partial \phi}{\partial n_+}(s) = -\frac{\sigma(s)}{2\epsilon_0} + \int_S \frac{\sigma(s')}{\epsilon_0} \frac{\partial G}{\partial n}(s \mid s')\, ds'. \tag{14b}$$

When $\phi(s)$ is defined over a closed curve S, then as a convention we use $\hat{n}_-$ when dealing with the interior of the region and $\hat{n}_+$ when concerned with the exterior region. If S is considered to be made up of two (or more) sections S_1 and S_2, as in Fig. 1, then one can define the normal directions along each section arbitrarily as long as $\hat{n}_1$ and $\hat{n}_2$ are in the same direction at any point. The arbitrariness is apparent because if the region is open or if S_1 and S_2 are separated (i.e., $\phi(s)$ is not defined over a closed curve) then one can presume the curve closed in various ways that will reverse the normal directions of one section with respect to the other. The portions that are added to affect the closure are of no consequence to the integration as the charge is zero along those paths. Generally then, one can think of $\hat{n}_-$ as the normal approaching S and $\hat{n}_+$ as the normal leaving S, the direction of travel being arbitrary.

Subtracting (14a) and (14b) one obtains

$$\frac{\partial \phi}{\partial n_-}(s) - \frac{\partial \phi}{\partial n_+}(s) = \frac{\sigma(s)}{\epsilon_0} \tag{15}$$

which is the well-known result describing the discontinuity of electric flux due to a surface charge distribution. As well as satisfying Laplace's equation everywhere not on S, due to the nature of the Green's function *any* $\sigma(s)$ will also satisfy this required relationship. The solution, however, will also satisfy the required boundary conditions.

By differentiating (13) with respect to the unprimed variable, it is clear that what (14) does is to add up all the contributions to $\partial\phi/\partial n$ at any observation point due to whatever free or polarization charge exists elsewhere and then to add to this the discontinuity due to the local charge.

To solve (13) we propose the new but entirely obvious strategy of writing the functional (4) with $u = \sigma$, $L = K$, and $f = g$. Thus

$$F = \langle K\sigma,\sigma \rangle - 2\langle \sigma,g \rangle \tag{16}$$

in which the inner product is defined as an integral over S. Note that at the solution point, the first term within the first pair of brackets is the potential $\phi(s)$ as per (13). The product of potential and charge integrated over the surfaces yields the energy of the system. The second inner product yields twice the energy. From an energy point of view, the parallel with the partial differential equation approach is exact.

From a numerical point of view, we shall seek a solution of the Fredholm integral equation by finding the stationary point of F with respect to certain variational parameters incorporated in the form of the approximation to $\sigma(s)$. For the solution to exist at a stationary point of F, we must show that K is self-adjoint. To prove that the functional and hence the error is minimized at a stationary point we must show that K is positive-definite as well. If these requirements can be satisfied, then the advantages of variational methods for partial differential equations should be available to the solution of the Fredholm integral equation of the first kind.

Making use of the symmetry of the Green's functions in s and s', it is easy to show that

$$\langle K\sigma,\tau \rangle = \langle \sigma,K\tau \rangle \tag{17}$$

which is the definition of the self-adjointness of K.

To prove positive-definiteness, note that

$$\langle K\sigma,\sigma \rangle = \int_S \left[\int_S \frac{\sigma(s')}{\epsilon_0} G(s \mid s')\, ds' \right] \sigma(s)\, ds$$

$$= \int_S \phi(s)\sigma(s)\, ds. \tag{18}$$

By virtue of (13), Green's first identity applied to the interior region is

$$\int_S \phi \frac{\partial \phi}{\partial n_-}\, ds = \iint_{\text{interior}} (\nabla\phi)^2\, dx\, dy + \iint_{\text{interior}} \phi \nabla^2\phi\, dx\, dy \tag{19a}$$

and over the exterior region

$$-\int_S \phi \frac{\partial \phi}{\partial n_+}\, ds = \iint_{\text{exterior}} (\nabla\phi)^2\, dx\, dy + \iint_{\text{exterior}} \phi \nabla^2\phi\, dx\, dy. \tag{19b}$$

The negative sign in (19b) is required because the normal required for Green's identity is opposite in direction to $\hat{n}_+$. As Laplace's equation is satisfied everywhere not on S, the integrals involving $\nabla^2\phi$ vanish. Thus adding (19a) and (19b) we obtain

$$\int_S \phi \left[\frac{\partial \phi}{\partial n_-} - \frac{\partial \phi}{\partial n_+}\right] ds = \iint_{\text{all space}} (\nabla\phi)^2 \, dx \, dy. \quad (20)$$

By virtue of (15), (20) becomes

$$\iint_{\text{all space}} \epsilon_0 (\nabla\phi)^2 \, dx \, dy = \int_S \phi\sigma \, ds. \quad (21)$$

This development parallels that of Tricomi [4].

Note that the surface integral in (19) is not shown to be over a closed contour. This is simply in recognition of the possibility that $\sigma(s)$ may not exist continuously over a closed path if, say, a conducting boundary does not close upon itself. With this in mind, the integral in (18) is the same as the one on the right-hand side of (21). Thus substitution of (21) into (18) yields

$$\langle K\sigma,\sigma\rangle = \iint_{\text{all space}} \epsilon_0 (\nabla\phi)^2 \, dx \, dy \quad (22)$$

which is clearly positive for nonzero ϕ. Hence, K is positive definite, (16) is minimized at the stationary point, and the rms error is the least attainable for any order of approximation. The above proof is essentially the same as one given earlier [12] but with moderate alterations including a slightly different notation.

The functional is

$$F = \int_S \int_S \sigma(s)\sigma(s') G(s \mid s') \, ds' \, ds - 2\int_S \sigma(s) g(s) \, ds \quad (23)$$

in integral form. An example will be presented in which $\sigma(s)$ will be approximated by a set of pulse functions of arbitrary amplitude and then by a polynomial with unknown coefficients. These variational parameters will be computed by finding those values that make F stationary.

B. The Interface Problem

Suppose a surface S divides all of space into two parts. To be specific, let one part be air and the other part a homogeneous dielectric of constant ϵ_r. It is well known that a constraint must be placed upon the normal derivatives on alternate sides of S. If the normal to the surface within the dielectric is $\hat{n}_-$, we have the constraint

$$\epsilon_r \frac{\partial \phi}{\partial n_-}(s) = \frac{\partial \phi}{\partial n_+}(s). \quad (24)$$

Equation (24) may be viewed as a special case of the most general mixed boundary-*cum*-interface condition

$$a_1 \frac{\partial \phi}{\partial n_-}(s) - a_2 \frac{\partial \phi}{\partial n_+}(s) + a_3\phi(s) = h(s) \quad (25)$$

where all $a_i \geq 0$. The developments of this section may easily be extended to handle (25).

We realize that in the absence of any free charge, the polarization charge vanishes if the material is not an electret. However, we shall proceed to develop a functional for the approximation of polarization charge to satisfy (24) omitting, for the moment, consideration of the inhomogeneous part of the equation. In the next section we shall see how the inhomogeneous part (or forcing function) finds its way into the statement of the overall problem.

Substituting (14) into (24), we obtain the operator equation

$$K\sigma(s) = \frac{\epsilon_r + 1}{2\epsilon_0}\sigma(s) + \frac{\epsilon_r - 1}{\epsilon_0}\int_S \sigma(s') \frac{\partial G}{\partial n}(s \mid s') \, ds' = 0. \quad (26)$$

It is necessary for K to be self-adjoint that

$$\frac{\partial G}{\partial n}(s \mid s') = \frac{\partial G}{\partial n'}(s \mid s'). \quad (27)$$

For general curves, the line from s to s' makes one angle with the normal to S at s and another angle at s'. Therefore, (27) holds only for certain specific curves and so K is not generally self-adjoint.

Define a modified integral operator K' by multiplying (26) by the Green's function and integrating over the surface. This yields

$$K'\sigma = \frac{\epsilon_r + 1}{2\epsilon_0}\int_S G(s \mid s'')\sigma(s) \, ds + \frac{\epsilon_r - 1}{\epsilon_0}\int_S \sigma(s') \int_S G(s \mid s'') \frac{\partial G}{\partial n}(s \mid s') \, ds \, ds' = 0. \quad (28)$$

If $K'\sigma = \langle K\sigma,G\rangle = 0$, then $K\sigma = 0$ if $G \neq 0$. Hence, a solution of (28) implies a solution of (26).

Application of Green's theorem to the two functions $G(s \mid s'')$ and $G(s \mid s')$, with integration in the unprimed coordinates, shows that

$$\int_S G(s \mid s'') \frac{\partial G}{\partial n}(s \mid s') \, ds = \int_S \frac{\partial G}{\partial n}(s \mid s'') G(s \mid s') \, ds \quad (29)$$

with this factor seen to be symmetric, it is easy to show that K' is a symmetric operator.

In order to prove positive-definiteness of K', note once again that any assumed σ will generate a field that satisfies (13) and (14) exactly. Through substitution one obtains

$$\langle K'\sigma,\sigma\rangle = \int_S \frac{\sigma(s'')}{\epsilon_0}\left\{\int_S G(s\mid s'')\left[\frac{\epsilon_r+1}{2}\sigma(s) + (\epsilon_r-1)\int_S \sigma(s')\frac{\partial \dot{G}}{\partial n}(s\mid s')\,ds'\right]ds\right\}ds''$$

$$= \int_S \frac{\sigma(s'')}{\epsilon_0}\left\{\int_S G(s\mid s'')\left[\epsilon_0\epsilon_r\frac{\partial\phi}{\partial n_-}(s) - \epsilon_0\frac{\partial\phi}{\partial n_+}(s)\right]ds\right\}ds''$$

$$= \int_S \epsilon_0\left(\epsilon_r\frac{\partial\phi}{\partial n_-}(s) - \frac{\partial\phi}{\partial n_+}(s)\right)\phi(s)\,ds. \tag{30}$$

Application of Green's first identity, as in (20), results in

$$\langle K'\sigma,\sigma\rangle = \epsilon_0\epsilon_r \iint_{\text{interior}} (\nabla\phi)^2\,dx\,dy + \epsilon_0 \iint_{\text{exterior}} (\nabla\phi)^2\,dx\,dy \geq 0 \tag{31}$$

and so the modified integral operator K' is positive-definite. Again we have energy minimization.

It is not surprising that one is able to obtain a symmetric and positive-definite form. After all, we began by using the operator defined by (13)—which satisfies these conditions—and included a constraint upon admissible trial functions $\sigma(s)$. The addition of a constraint, even with amendment of the functional, should not destroy symmetry and positive-definiteness irrevocably.

The functional, i.e., the first line of (30), may appear somewhat formidable due to the presence of a triple surface integral. However, no new singularities are introduced as the derivative of the Green's function is not singular for smooth S. It behaves as

$$\lim_{s\to s'}\frac{\partial G}{\partial n}(s\mid s') = 0. \tag{32}$$

The general boundary condition (25) can be formulated as the Euler equation of a functional for a positive-definite operator by following essentially the same procedure.

C. *Mutually Constrained Finite Elements*

Refer again to the Dirichlet problem. For a surface S, the potential $\phi(s) = g(s)$ is specified and one must find $\sigma(s)$. Let us arbitrarily consider the surface to be divided into two parts S_1 and S_2. Given $\phi(s_1) = g(s_1)$ and $\phi(s_2) = g(s_2)$, it is required to find $\sigma(s_1)$ and $\sigma(s_2)$.

Imagine that $\sigma(s_2)$ is suppressed. (For clarity, think of the original $\sigma(s_2)$ as being known.) With $\sigma(s_2) = 0$, the boundary condition on S_1 must be amended to

$$g(s_1) - \int_{s_2}\frac{\sigma(s_2)}{\epsilon_0}G(s_1\mid s_2)\,ds_2$$

$\sigma(s_2)$ within the integral is understood to be the charge distribution on S_2 that existed prior to its removal. Also, the boundary condition on S_2 must become

$$g(s_2) - \int_{s_2}\frac{\sigma(s_2')}{\epsilon_0}G(s_2\mid s_2')\,ds_2'$$

in order to sustain $\sigma(s_2) = 0$. One can then write the functional

$$F_1 = \int_{s_1}\sigma(s_1)\int_{s_1}\frac{\sigma(s_1')}{\epsilon_0}G(s_1\mid s_1')\,ds_1'\,ds_1 - 2\int_{s_1}\sigma(s_1)\left[g(s_1) - \int_{s_2}\frac{\sigma(s_2)}{\epsilon_0}G(s_1\mid s_2)\,ds_2\right]ds_1. \tag{33}$$

Because $\sigma(s_2) = 0$, the integral over S_2 vanishes.

Note that the first double integral in (33) is the one that contains the variational parameters used to define $\sigma(s_1)$ over one element. They have been isolated within the functional appropriate to the same element. We indicate that the functional (33) pertains to element S_1 by denoting it F_1. We can differentiate with respect to each variational parameter and then set the result to zero. If, as is the usual method, the variational parameters enter linearly into $\sigma(s_1)$, then we can differentiate F_1 with respect to each of them and set the result to zero. Inspection of (33) will confirm that we obtain a set of linear equations.

If $\sigma(s_2)$ were actually known, then one could solve for $\sigma(s_1)$. However, $\sigma(s_2)$ is not known and so (33) produces a set of equations expressing $\sigma(s_1)$ in terms of $\sigma(s_2)$. Following the same procedure for the second element (and as many more as may be considered), another set of equations is generated and the whole system may then be solved simultaneously. It is interesting to note that the system of equations is identical to that obtained by a formal finite-element solution of (23) with $\sigma(s)$ represented by $\sigma(s_1)$, $\sigma(s_2)$, and so on.

This approach can be, but is rarely, used in the finite-element solution of partial differential equations. One could minimize the functional for each of a set of disconnected elements separately and only then add the constraints between elements. Usually, however, the constraints are built in at the outset by forcing continuity of potential across element boundaries.

We have considered (33) from the viewpoint of a Dirichlet problem with $\sigma(s_2)$ on a boundary whose potential is specified. Equation (33) is more general than that and $\sigma(s_2)$ may be polarization charge located at the surface of a dielectric, say.

Now we consider the effect of free and/or polarization charge upon a functional written for an interface S_1. Generalizing (26), we obtain

$$K\sigma(s) = \frac{\epsilon_r + 1}{2\epsilon_0}\sigma(s) + \frac{\epsilon_r - 1}{\epsilon_0}\int_{S_1}\sigma(s_1')\frac{\partial G}{\partial n}(s_1 \mid s_1')\,ds_1'$$

$$= -\frac{\epsilon_r - 1}{\epsilon_0}\int_{S_2}\sigma(s_2')\frac{\partial G}{\partial n}(s_1 \mid s_2')\,ds_2' \qquad (34)$$

where the right-hand side represents the contribution from a known $\sigma(s_2)$.

Thus we have an inhomogeneous asymmetric operator equation. Now, making the operator symmetric in the same way as for (28) we find that

$$K'\sigma(s_1') = \frac{\epsilon_r + 1}{2\epsilon_0}\int_{S_1} G(s_1 \mid s_1')\sigma(s_1)\,ds_1$$

$$+ \frac{\epsilon_r - 1}{\epsilon_0}\int_{S_1}\sigma(s_1'')\int_{S_1} G(s_1 \mid s_1'')$$

$$\cdot\frac{\partial G}{\partial n}(s_1 \mid s_1'')\,ds_1\,ds_1''$$

$$= -\frac{\epsilon_r - 1}{\epsilon_0}\int_{S_2}\sigma(s_2'')\int_{S_1} G(s_1 \mid s_1'')$$

$$\cdot\frac{\partial G}{\partial n}(s_1 \mid s_2'')\,ds_1\,ds_2''. \qquad (35)$$

We may now write a functional from which we can obtain a set of equations expressing $\sigma(s_1)$ in terms of $\sigma(s_2)$ as with the Dirichlet example above.

We have not been able to find a quadratic functional, defined over all of S, which produces, upon application of the formal finite-element method, different types of boundary conditions on different parts of S. Generally, a linear combination of the different boundary conditions results at all points of S, with the specified boundary conditions being satisfied only with $\phi\,\partial\phi/\partial n = 0$ at all points of s. The method of mutually constrained finite elements, on the other hand, produces solutions with the specified boundary conditions, and furthermore degenerates to identically the formal finite-element method when the boundary conditions on different parts of S are all of the same type.

III. Examples

Several computational difficulties arise when one actually begins to solve problems with these integral-equation functionals. Mention has been made of the Green's function singularity which, as we will show by example, may be treated with only minor inconvenience. There is also the problem of singular charge distributions which arise, for instance, at edges and corners of conductors. Taken by itself, such a singularity poses no major difficulties. However, when charge singularities occur simultaneously with Green's function singularities, very particular care must be taken. Problems such as these are not insuperable. As experience is gained in solving them, they will tend to appear fairly routine in time.

Two examples are presented. The square parallel plate capacitor problem is solved using the logarithmic Green's function (10) and the surface S is one dimensional. This example may be compared to the transform method of Yamashita [18]. The algorithms for integrating the singular functions are presented in detail. The three-dimensional problem is representative of a section of microstrip line, with a discontinuity, or part of printed circuit board. The three-dimensional Laplace Green's function is used, hence the solution is quasi-static, and the surface S is two dimensional.

A. The Square Parallel-Plate Capacitor

Consider two very long thin parallel conducting strips, as shown in Fig. 3, with a potential difference of 2 V. It is known [13] that the capacitance of this configuration in the MKS system is 18.7 pF/m.

By nature of the symmetries of the problem, we may write the Fredholm equation as

$$1 = \int_0^1 \frac{\sigma(x')}{\epsilon_0} G(x,1 \mid x',1)\,dx' \qquad (36)$$

where the Green's function is obtained by images from (10). Here, then, we have

$$G(x,y \mid x',1) = \frac{-1}{2\pi}\ln\left(\frac{[(x-x')^2+(y-1)^2][(x+x')^2+(y-1)^2]}{[(x-x')^2+(y+1)^2][(x+x')^2+(y+1)^2]}\right)^{1/2} \qquad (37)$$

and the Dirichlet functional to solve this problem is, from (16)

$$F(\sigma) = \frac{1}{\epsilon_0}\int_0^1\sigma(x)\int_0^1\sigma(x')G(x,1 \mid x',1)\,dx'\,dx - 2\int_0^1\sigma(x)\,dx. \qquad (38)$$

It is known [14] that the charge distribution has a singularity at the edge of the plate which may be written as

$$\sigma(x) \simeq \frac{1}{(1-x)^{1/2}}. \qquad (39)$$

We consider the charge to be given by a combination of n pulse functions [Fig. 2(a)] together with a polynomial function with the inclusion of the singularity (39). Then we have on the plate

$$\phi(x) = \frac{1}{\epsilon_0}\sum_{i=1}^{n}\left(\sigma_i\int_{x_i-h/2}^{x_i+h/2} G(x,1 \mid x',1)\,dx'\right) + \frac{1}{\epsilon_0}\sum_{j=0}^{m} a_j\int_0^1\frac{x'^j G(x,1 \mid x',1)\,dx'}{(1-x')^{1/2}} \qquad (40)$$

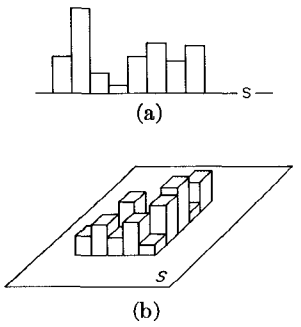

Fig. 2. (a) Pulse functions in one dimension. (b) Pulse functions in two dimensions.

where $h = 1/n$, n being the number of pulse functions, and m being the order of the polynomial approximation. If there are no pulse functions ($n = 0$), the first term of (40) is simply not computed. If there is to be no singular function in the approximation ($m = 0$), the second term of (40) is not computed. The σ_i, the pulse heights, and the a_j, the polynomial coefficients, are the variational parameters. They total $n + m$.

Substituting (40) into (38) and taking derivatives with respect to the variational parameters results in the following system of equations:

$$\frac{1}{\epsilon_0}\sum_{i=1}^{n}\sigma_i\int_{x_i-h/2}^{x_i+h/2}\int_{x_k-h/2}^{x_k+h/2}G(x,1\mid x',1)\,dx'\,dx + \frac{1}{\epsilon_0}\sum_{j=0}^{m}a_j\int_{x_k-h/2}^{x_k+h/2}\int_0^1\frac{x'^jG(x,1\mid x',1)}{(1-x')^{1/2}}\,dx'\,dx = h, \qquad k = 1,n \quad (41a)$$

and

$$\frac{1}{\epsilon_0}\sum_{i=1}^{n}\sigma_i\int_{x_i-h/2}^{x_i+h/2}\int_0^1\frac{x'^kG(x,1\mid x',1)}{(1-x')^{1/2}}\,dx'\,dx + \frac{1}{\epsilon_0}\sum_{j=0}^{m}a_j\int_0^1\frac{x^k}{(1-x)^{1/2}}\int_0^1\frac{x'^jG(x,1\mid x',1)}{(1-x')}\,dx'\,dx = \int_0^1\frac{x^k\,dx}{(1-x)^{1/2}} \qquad k = 0\cdots m. \quad (41b)$$

The double integrals in (41) are computed by standard Gaussian quadrature techniques [15], with special handling of the singularities. There are four singular integrals to be examined. First of all, the right-hand side of (41b) is

$$\int_0^1\frac{x^k}{(1-x)^{1/2}}\,dx = \frac{2k}{(2k+1)}\int_0^1\frac{x^{k-1}}{(1-x)^{1/2}}\,dx$$

and

$$\int_0^1\frac{dx}{(1-x)^{1/2}} = 2. \quad (42)$$

Therefore, this integral can be computed analytically.

The other singular integrals involve the Green's function (37) where only one member of the numerator within the root vanishes.

The following general technique is used for the computation. We assume, for example that $I = \int_a^b g(x)\,dx$ converges and that g is singular at $x = a$, and behaves like $h(x)$ when $\int_a^b h(x)\,dx$ can be calculated analytically. We then write

$$I = \int_a^b [g(x) - h(x)]\,dx + \int_a^b h(x)\,dx. \quad (43)$$

The first integral of (43) no longer is singular and is computed by Gaussian quadrature, with the second integral obtained analytically.

To handle the Green's function singularity we subtract the singular part $G_s(x \mid x')$ from the Green's function leaving a regular function $G_r(x,1 \mid x',1)$. From (37) we have

$$G_s(x \mid x') = -\frac{1}{2\pi}\ln\mid x - x'\mid \quad (44)$$

and

$$G_r(x,1 \mid x',1) = G(x,1 \mid x',1) - G_s(x \mid x'). \quad (45)$$

The first integral of (41a) is singular when $i = k$. We perform the integration in two steps, the *last* step being

$$\int_{x_i-h/2}^{x_i+h/2}f(x')\,dx'. \quad (46)$$

The regular function $f(x')$ is obtained by applying (43), using (44) and (45), as follows:

$$f(x') = \int_{x_i-h/2}^{x_i+h/2}G_r(x,1 \mid x',1)\,dx + \int_{x_i-h/2}^{x_i+h/2}G_s(x \mid x')\,dx. \quad (47)$$

The first integral in (47), and that in (46) are computed numerically. The last integral of (47) is obtained analytically

$$\int_a^b G_s(x \mid x')\,dx = \frac{-1}{2\pi}[(x'-a)\ln(x'-a) + (b-x')\cdot\ln(b-x') + a - b]. \quad (48)$$

The second integral of (41a) is written

$$\int_0^1\frac{x'^j}{(1-x')^{1/2}}[f(x') - f(1)]\,dx' + f(1)\int_0^1\frac{x'^j\,dx'}{(1-x')^{1/2}}. \quad (49)$$

The regular function $f(x')$ is obtained as before (47).

The last integral on the left side of (41b) is written similarly to (49), where here

$$f(x') = \int_0^1\frac{x^kG(x,1 \mid x',1)\,dx}{(1-x)^{1/2}}. \quad (50)$$

The singularities at $x = x'$, $x = 1$, $x' = 1$ are handled by integrating (50) as

$$f(x') = \int_0^1 \left\{ \frac{x^k}{(1-x)^{1/2}} [G_r(x,1 \mid x',1) - G_r(1,1 \mid x',1)] + G_s(x \mid x') \left[\frac{x^k - 1}{(1-x)^{1/2}} - \frac{x'^k - 1}{(1-x')^{1/2}} \right] \right\} dx + G_r(1,1 \mid x',1) \int_0^1 \frac{x^k\, dx}{(1-x)^{1/2}} + \frac{x'^k - 1}{(1-x')^{1/2}} \cdot \int_0^1 G_s(x \mid x')\, dx + \int_0^1 \frac{G_s(x \mid x')\, dx}{(1-x)^{1/2}}. \quad (51)$$

The first integral of (51) is computed numerically, and the last integral is obtained analytically

$$\int_0^1 \frac{G_s(x \mid x')\, dx}{(1-x)^{1/2}} = \frac{1}{\pi} \left[2 - \ln (x') + (1-x')^{1/2} \cdot \ln \left\{ \frac{1 - (1-x')^{1/2}}{1 + (1-x')^{1/2}} \right\} \right]. \quad (52)$$

Three experiments are presented with various combinations of pulse functions and polynomial singular functions. For the configuration of the capacitor we have chosen, the capacitance is obtained simply as the total charge on the plate (0,1), or as the negative of the value of the functional (38) at the solution point.

The first experiment is without singular functions [$m = 0$ in (40)]. Table I lists the number of pulses used and shows convergence of the capacitance and the potential at an arbitrary point in the plane. It should be noted that convergence is monotonic.

For the second experiment we add one singular function to the pulse functions [$m = 1$ in (40)]. Table II shows that with the one singular function alone, one unknown in the system-capacitance and field values within one percent are achieved. The capacitance is seen to converge with the addition of one pulse whereas four pulses are required before the field converges. This is to be expected, since the energy method implies faster convergence of the energy than the field.

TABLE I
CAPACITOR—PULSES ALONE

number of pulses	capacitance pf/m	$\phi(\frac{40}{9}, 10)$
1	17.72	.1063
2	18.20	.1092
5	18.51	.1110
10	18.62	.1117
20	18.68	.1121
30	18.70	.1122
40	18.71	.1123
50	18.72	.1124

TABLE II
CAPACITOR—ONE SINGULAR FUNCTION WITH PULSES

number of pulses	number of unknowns	capacitance pf/m	$\phi(\frac{40}{9}, 10)$
0	1	18.57	.1115
1	2	18.72	.1123
4	5	18.72	.1124
9	10	18.72	.1124

For the third experiment the polynomial order m in (40) is varied with no pulse functions [$n = 0$ in (40)]. The results, presented in Table III, are somewhat better than those obtained in the second experiment (Table II) largely due to the fact that each trial function here is singular, containing $(1-x)^{1/2}$ in the denominator. Equipotentials are plotted in Fig. 3.

The importance of including special functions to handle the known behavior of solution singularities cannot be underestimated. Reduction by factors of 10 and 20 in the number of unknowns required for a specified accuracy is apparent from the tables. Two ways of implementing singular functions have been demonstrated as well. A separate independent singular function with its own variational parameter can be used, as in the second experiment, or all the trial functions can be made singular, as in the third experiment. The results we obtained indicate that if the singularity representation is accurate, better

TABLE III
CAPACITOR—POLYNOMIALS WITH SINGULAR TERM

order of polynomial	number of unknowns	capacitance pf/m	$\phi(\frac{40}{9}, 10)$
0	1	18.57	.1115
1	2	18.72	.1124
2	3	18.72	.1124
3	4	18.72	.1124

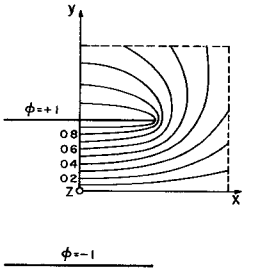

Fig. 3. Square capacitor problem—cross section at $z = 0$.

results are achieved if all the trial functions are made singular. However, if the singularity is not well known, it may be better to introduce a separate singular trial function, which the variational method can use "as needed" in producing a solution.

B. Microstrip—A Three-Dimensional Problem

Consider a square slab ($4 \times 4 \times 1$) of homogeneous dielectric (constant ϵ_r) lying on an infinite ground conductor in the $z = 0$ plane. On top of this slab we place a T-shaped thin conductor at unit potential as shown in Fig. 4. We seek the electrostatic field. The problem is representative of a microstrip line discontinuity, or a printed circuit board with a TEM quasi-static approximation to the time-varying fields.

To obtain the electrostatic solution we will use square equal area pulse functions for the charge distribution on the top conductor and the air–dielectric interface, with a separate singular function defined over the top conductor to handle known solution singularities. The approach parallels that used in the second experiment of Section III-A above.

The symmetries allow us to seek solution in the region of space $y \geq 0$, $z \geq 0$, with an amended free-space Green's function constructed by images from (11):

$$G(r \mid r') = G(x,y,z \mid x',y',z')$$
$$= \frac{1}{4\pi}\left\{\frac{1}{((x-x')^2+(y-y')^2+(z-z')^2)^{1/2}}\right.$$
$$+\frac{1}{((x-x')^2+(y+y')^2+(z-z')^2)^{1/2}}$$
$$-\frac{1}{((x-x')^2+(y-y')^2+(z+z')^2)^{1/2}}$$
$$\left.-\frac{1}{((x-x')^2+(y+y')^2+(z+z')^2)^{1/2}}\right\}. \tag{53}$$

We remove the dielectric and place a polarization charge on the interface surface S_I, and demand that the interface condition (24) hold on the surfaces of the slab $x = 0$, $y = 2$, $x = 4$ and on the top of the dielectric ($z = 1$) where the conductor is not present (in each case $y \geq 0$).

On the conducting plate surface at $y = 1$, S_P, we place a charge equal to the real charge required to maintain the potential less the polarization charge under the conductor. That is, we seek the *net* charge on the conductor.

Alternately, we could have taken S_I to have included all the surface $z = 1$, $y \geq 0$ and superimposed S_P, in which case we would have obtained, on the plate, both the real charge and the polarization charge. We chose the former method, simply because fewer unknowns would result.

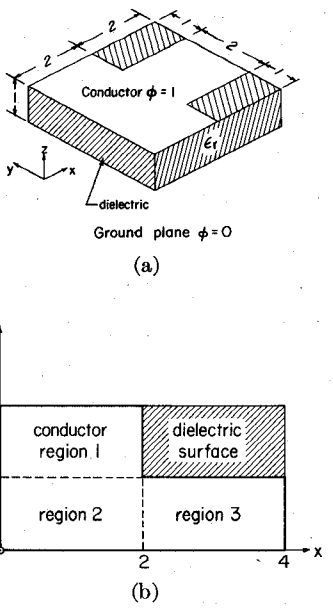

Fig. 4. (a) Microstrip problem configuration. (b) Microstrip problem top view.

Following the method outlined in Section II-C, we write the Dirichlet functional for the plate surface S_P and the interface functional for S_I. We then differentiate each functional with respect to the variational parameters and solve the systems of equations simultaneously.

To represent the charge on the surfaces we use square equal-area pulse functions [Fig. 2(b)] denoting the ith pulse region by Δ_i, on both S_P and S_I. Further, we introduce a single singular function f_s defined on the plate S_P to handle edge and corner singularities. We shall discuss the choice of this singular function shortly. To simplify the notation, we take the first m pulses to lie on the plate and the remaining pulses to lie on the interface. That is, the pulses on the plate S_P are given by

$$\Delta_i, \qquad i = 1 \cdots m \tag{54a}$$

and the pulses on the interface S_I are given by

$$\Delta_i, \qquad i = m+1 \cdots n. \tag{54b}$$

Thus in total, we have n pulses and one singular function. As in the first example, we denote the height of the pulse in region Δ_i by σ_i, and the coefficient of the singular function by a, giving us $n+1$ variational parameters, the σ_i, and a.

The potential, then, is given by

$$\phi(r) = \sum_{i=1}^{n} \frac{\sigma_i}{\epsilon_0} \int_{\Delta_i} G(r \mid r')\, ds' + \frac{a}{\epsilon_0} \int_{S_P} f_s(r') G(r \mid r')\, ds'. \tag{55}$$

Substituting (55) into the Dirichlet functional for S_P and taking derivatives with respect to the pulse height parameters on the plate (54a) results in the system of equations

$$\sum_{i=1}^{n} \frac{\sigma_i}{\epsilon_0} \int_{\Delta_j} \int_{\Delta_i} G(r \mid r')\, ds'\, ds + \frac{a}{\epsilon_0} \int_{\Delta_j} \int_{S_P} f_s(r') G(r \mid r')\, ds'\, ds = \int_{\Delta_j} ds, \qquad j = 1 \cdots m. \quad (55a)$$

Taking the derivative with respect to a results in the single equation

$$\sum_{i=1}^{n} \frac{\sigma_i}{\epsilon_0} \int_{\Delta_i} \int_{S_P} f_s(r') G(r \mid r')\, ds'\, ds + \frac{a}{\epsilon_0} \int_{S_P} \int_{S_P} f_s(r)\, f_s(r') G(r \mid r')\, ds'\, ds = \int_{S_P} f_s(r)\, ds. \quad (55b)$$

We generate the remaining equations by substituting (55) into the interface functional for S_I, derived from (35) and taking derivatives with respect to the pulse height parameters σ_i on the interface, for $i = m + 1 \cdots n$. We obtain

$$\sum_{k=m+1}^{n} \sum_{i=1}^{n} \frac{(\epsilon_r' - 1)}{\epsilon_0} \sigma_i \int_{\Delta_i} \int_{\Delta_j} \int_{\Delta_k} G(r \mid r'') \frac{\partial G}{\partial n}(r \mid r') \cdot ds\, ds''\, ds' + \sum_{k=m+1}^{n} \sum_{i=m+1}^{n} \left(\frac{\epsilon_r + 1}{2\epsilon_0} \right) \cdot \sigma_i \int_{\Delta_i} \int_{\Delta_j} G(r \mid r')\, ds\, ds' + \sum_{k=m+1}^{n} \left(\frac{\epsilon_r - 1}{\epsilon_0} \right) \cdot a \int_{\Delta_j} \int_{S_P} f_s(r') \int_{\Delta_k} G(r \mid r'') \frac{\partial G}{\partial n}(r \mid r')\, ds\, ds'\, ds'' = 0, \qquad j = m + 1 \cdots n. \quad (55c)$$

Equations (55a)–(55c) now give us a system of $n + 1$ equations in $n + 1$ unknowns which are solved simultaneously to obtain the σ_i and a.

The method used to perform the integrations follows identically the procedure used for the previous example—Gaussian quadrature with subtraction and addition of singular terms, as in the discussion regarding (43). Although the integrations here are clearly more complicated, the algorithms remain straightforward.

Some difficulty is encountered in selecting an appropriate singular function. From the paper by Braunbek [16] it appears as though at a great distance from a corner, the edge condition used in the capacitor example above is appropriate. Near a corner the situation is unclear. Referring to Fig. 5, where R_1 is the distance perpendicular from the edge, and R_2 is the distance along the edge from the corner, it appears that we can express, locally,

$$f_s(r) = \frac{1}{R_1^{P(R_2,\theta)}}. \quad (56)$$

The function $P(R_2,\theta)$ is not known and, as Braunbek pointed out, the results he obtained were not exactly solutions of the differential equation. We decided to select an arbitrary function, continuous over the plate, which could be integrated fairly easily, and which produced as nearly constant a potential over the plate as possible. This criterion is reasonable, since f_s is a first approximation to the exact singular distribution which should produce exactly a constant potential on the plate.

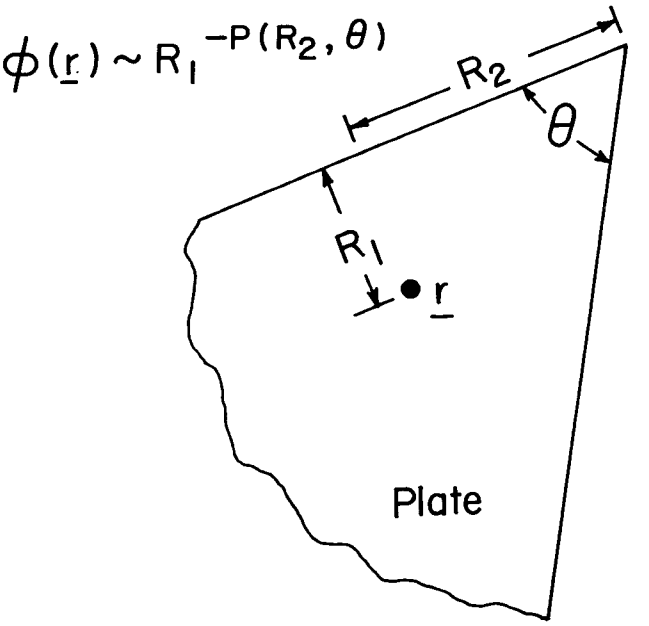

Fig. 5. Singular function representation near a corner.

Referring to the three regions of the plate, in Fig. 4(b), we chose in region 1

$$f_s(x,y) = \frac{1}{[x(2-x)(2-y)]^P} \quad (57a)$$

in region 2

$$f_s(x,y) = \frac{1}{[x(3-x-y)]^P} \quad (57b)$$

in region 3

$$f_s(x,y) = \frac{1}{[(4-x)(1-y)]^P}. \quad (57c)$$

Experiments were conducted to determine the optimum value of P—which we required to be constant. We found $P = \frac{1}{4}$ produced the least perturbation of potential over the plate—of the order of 10-percent variation. Some of Braunbek's results can be interpreted to say that $P = \frac{1}{4}$ is valid for a right-angle external corner, of which we have three. Interestingly enough, the 10-percent variation occurred mainly near the internal corner, at (2,1,1), where Braunbek comments that the charge is nonsingular.

In any case, *no harm can be done by introducing* (57) *as the singular function.* If it is of no help, the variational scheme will merely ignore it. In other computational schemes, it could make matters worse.

If we take $\epsilon_r = 1$ we can ignore all charge on the interface S_I since it must vanish. Accordingly, experiments were done with $\epsilon_r = 1$ to investigate the convergence properties of the scheme, and to determine the effect of

the approximate singular function (57). Since we asked that the pulses be square, the number of pulses required is $6N^2$, $N = 1,2,3,4$, for the plate alone. With $N = 4$ there are 96 pulse functions on the plate alone, and this is about the limit, due to ill conditioning of the very dense matrix we produce.

Table IV shows results for the pulse functions alone. It is to be noted that convergence is monotonic with the capacitance value (MKS) being approached from below as expected. Table V shows the effect of including the singular function along with the pulses. Clearly, the singular function helps, but convergence is not nearly as fast as in the previous problem. The column giving the percentage of capacitance due to the singular function tells why: the method relies more upon the pulse functions when they are available than it does on an incorrect singular function. Clearly, from Table II, it is clear that the singularity plays a more prominent role. Two things are immediately apparent: inclusion of the singular function helps; and the singular function is not correct.

The final results presented are from an experiment done with $\epsilon_r = 10$. Due to our initial restriction that the pulse regions be square, the number of pulses required is $16N^2$, $N = 1,2$. With $N = 2$ we have 64 pulse functions, giving us a total of 65 unknowns. The next possibility, with $N = 3$ gives us 145 unknowns, and the matrix in this case was found to be very ill conditioned. Thus the results are presented with $N = 2$. Fig. 6 shows equipotential cross sections of the resulting field. These results must be taken as preliminary, and quite approximate (1- or 2-percent error). From Table V, without the polarization charges, but with a singular function, it is seen that the field has not yet converged with $N = 2$. Selection of a better singular function, and better finite surface element representation, using polynomial functions will no doubt greatly improve things.

TABLE IV
MICROSTRIP PROBLEM—$\epsilon_r = 1$—PULSES ALONE ON PLATE

N	number of pulses	capacitance pf	$\phi(2, 3, 2)$
1	6	119.4	.1968
2	24	125.6	.2064
3	54	127.8	.2102
4	96	129.2	.2127

TABLE V
MICROSTRIP PROBLEM—$\epsilon_r = 1$—ONE SINGULAR FUNCTION + PULSES

N	number of pulses	number of unknowns	capacitance pf	$\phi(2,3,2)$	% capacitance from f_s
0	0	1	124.6	.2060	100.0
1	6	7	126.2	.2078	78.2
2	24	25	128.0	.2108	51.3
3	54	55	129.5	.2131	34.1
4	96	97	130.3	.2142	7.8

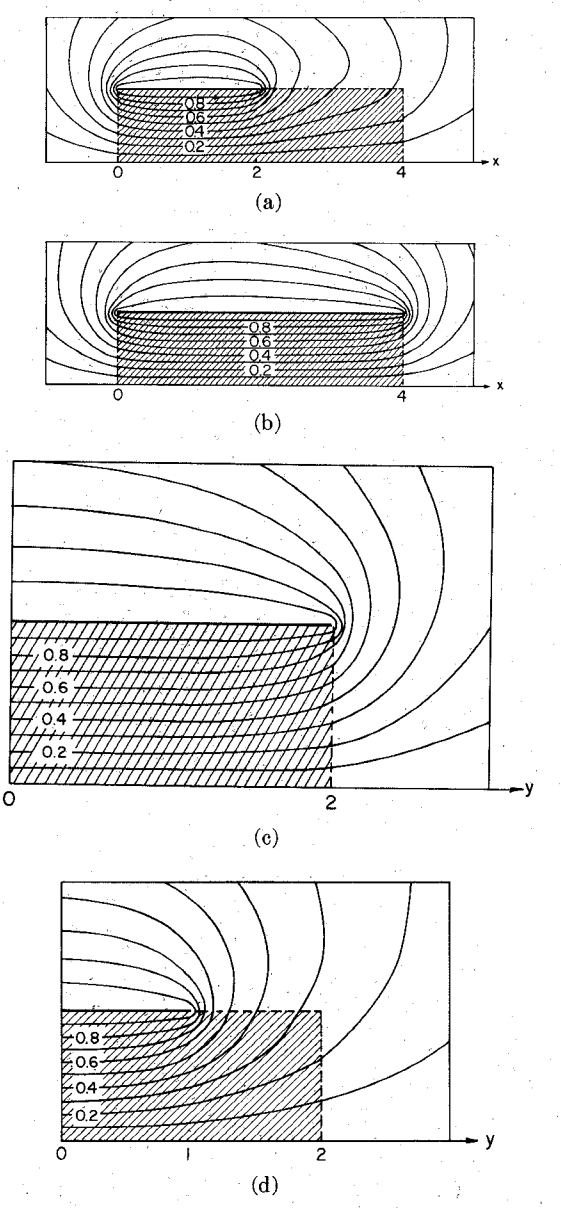

Fig. 6. Microstrip problem equipotential plots. (a) Cross section at $y = 0.5$. (b) Cross section at $y = 1.5$. (c) Cross section at $x = 1.0$. (d) Cross section at $x = 3.0$.

CONCLUSIONS

This paper has presented three basic concepts as follows.

1) The variational solution of the Fredholm integral equation of the first kind.

2) The implementation of mutually coupled finite elements in order to cope with various boundary conditions within one problem.

3) The use of free-space Green's functions rather than special ones.

In the pure Dirichlet problem the resulting equations using subdivision turn out to be those obtained without element subdivision. However, the method is very important as a vehicle for generating functionals, and the resulting matrices, for more complicated problems.

The method of constraints upon a variational solution was demonstrated in another context [17]. In that paper, a free-space problem, posed in terms of a partial differen-

tial equation, was solved within an arbitrary finite region with integral constraints placed upon the boundary in order to represent free space. There is no reason that one should not solve part of a problem variationally with a partial differential equation, another part variationally with an integral equation, and the two mutually constrained to yield a unique solution. Thus for any region the appropriate method can be used.

The application of the variational solution of integral equations, particularly in terms of coupled functionals, is an approach that the authors believe to be entirely novel. It turns out, in the pure Dirichlet problem with a homogeneous medium, that the resulting equations are exactly those obtained by the Galerkin scheme. Therefore, this equivalence constitutes a proof of convergence of the Galerkin scheme in this case. It seems unlikely, however, that the usual form of the Galerkin scheme has ever been used to generate equations for problems with interfaces and several boundary conditions. However, there seems to be no reason that the Galerkin method cannot be similarly formulated.

Of principal importance to future work, the problem of complex operators is paramount. By the simple act of converting a Helmholtz differential equation to its integral form, one transforms a real differential operator (assuming no losses) into a complex operator due to the term $e^{jk \cdot r}$ in the Green's function.

One then loses a guarantee of convergence, but some preliminary experience (with complex differential operators) in lossy media appears quite promising. There is a possibility that error bounds could be placed upon such formulations.

As numerical techniques permit the solution of practical three-dimensional problems, the corner (as distinct from the edge) field singularity will need a satisfactory resolution. We suggest that it may be feasible to discover the form of the local charge distribution through a variational study. Possibly, as an ancillary program, the computer could define the form at corner singularities prior to beginning the main computation.

This paper, which is somewhat imperfect and tentative in places, is intended as a "door-opener" to further study of what the authors believe to be a very promising approach.

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