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THE METHOD OF CONJUGATE GRADIENTS FOR THE NUMERICAL SOLUTION OF LARGE-BODY ELECTROMAGNETIC SCATTERING PROBLEMS

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Over the past few decades, many techniques have been developed for the numerical solution of integral equations representing electromagnetic scattering problems. However, a majority of these techniques are limited to electrically small scatterers, i.e., below the resonance range. This is primarily because the amont of CPU computer time and storage requirements become prohibitive for large body scatterers. Recent work indicates that a procedure based on the iterative conjugate gradient method can be incorporated into conventional numerical methods in order to extend the range of application of the techniques to larger geometries. In this paper we discuss the conjugate gradient method and illustrate several ways in which it can be applied to electromagnetic scattering problems. The discussion includes mention of the method as compared to conventional approaches as well as some of its limitations. In many practical scattering problems of interest at optical wavelengths, the method can provide a convenient means of treating problems which are electrically more than an order of magnitude larger than can be handled by other techniques.

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THE METHOD OF CONJUGATE GRADIENTS FOR THE NUMERICAL SOLUTION OF LARGE-BODY ELECTROMAGNETIC SCATTERING PROBLEMS

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ABSTRACT

Over the past few decades, many techniques have been developed for the numerical solution of integral equations representing electromagnetic scattering problems. However, a majority of these techniques are limited to electrically small scatterers, i.e., below the resonance range. This is primarily because the amount of CPU computer time and storage requirements become prohibitive for large body scatterers. Recent work indicates that a procedure based on the iterative conjugate gradient method can be incorporated into conventional numerical methods in order to extend the range of application of the techniques to larger geometries. In this paper we discuss the conjugate gradient method and illustrate several ways in which it can be applied to electromagnetic scattering problems. The discussion includes mention of the advantages of the method as compared to conventional approaches as well as some of its limitations. In many practical scattering problems of interest at optical wavelengths, the method can provide a convenient means of treating problems which are electrically more than an order of magnitude larger than can be handled by other techniques.

1. INTRODUCTION

The numerical solution of integral equations is an invaluable technique for the treatment of electromagnetic scattering problems. Asymptotic techniques, such as the Geometric Theory of Diffraction (GTD) and its extensions [1], have also been employed for solving high-frequency scattering problems. However, this method is not well-suited for dealing with scatterers that cannot be conveniently described in terms of a limited number of canonical geometries for which analytical diffraction coefficients are available. Furthermore, the GTD is not very useful for determining the near-field behavior and cannot be applied to many practical problems dealing with inhomogeneous or lossy scatterers. An additional difficulty with this type of asymptotic approach is that it may be impossible to estimate the accuracy of numerical results based on such techniques. Integral equations, on the other hand, can be formulated for scatterers of arbitrary shape [2], [3], [4]. Although few integral equations can be solved exactly, numerical solutions are readily obtained by a systematic application of techniques such as the method of moments (MoM) [3] - [6]. However, in the past, the application of this approach has been limited to bodies that are electrically small. The reason for this limitation will be evident from the discussion below.

The moment-method procedure involves replacing the unknown in the integral equation by N basis functions and reduces the problem to the solution of an N-th order matrix equation. In most problems, the unknown density needed for accuracy is at least ten per linear wavelength. Thus, computer time and memory requirements place an upper limit on the size of the body to be analyzed. This is especially true at optical wavelengths where the size of the scatterer is often comparable to or larger than the wavelength of the illumination source.

Current research in computational electromagnetics includes efforts to develop more efficient algorithms for the solution of integral equations, thereby permitting the analysis of electrically larger and more complex geometries. Because of their potential for efficiency and low storage requirements, iterative methods are often incorporated into these algorithms [7].

In this paper, we review one such iterative technique, viz., the method of conjugate gradients [8], which has been found useful for the solution of large body scattering problems. Although this technique was introduced by Hestenes and Stiefel more than thirty years ago for the iterative solution of matrix equations, it has only recently been applied extensively to electromagnetic scattering problems [9] - [19]. Recent work has clarified the advantages and the limitations of the method and has shown that the conjugate gradient method can, in many cases, be used to solve practical problems which cannot easily be treated by the conventional, direct solution of matrix equations.

The following section presents the conjugate gradient algorithm and identifies important features of the method. The remainder of the article presents examples to illustrate a number of different ways in which the method can be applied in practice.

2. THE CONJUGATE GRADIENT METHOD

Hestenes and Stiefel introduced the conjugate gradient method in 1952 [8]. Since then, it has received much use in engineering and applied mathematics [20] - [23]. Although the method can be applied to a quadratic functional on a general Hilbert space H, for our purposes it is sufficient to consider specifically Euclidean space E_N. For this space, the inner product and norm are defined in the usual manner:

$$\langle f,g \rangle = g^* f \tag{1}$$

$$||f|| = (\langle f,f \rangle)^{1/2} \tag{2}$$

The asterisk in Equation (1) denotes the transpose-conjugate matrix.

We wish to solve the linear system

$$LJ = E \tag{3}$$

where E is a known N-dimensional vector, J is an unknown N-dimensional vector, and L is a nonsingular N × N matrix. Let $\{P_i\}$ be a set of N linearly independent vectors in E_N. The unknown vector J can be represented as

$$J = \alpha_1 P_1 + \alpha_2 P_2 + \ldots + \alpha_N P_N \tag{4}$$

If the P-vectors are constrained to satisfy the orthogonality requirement

$$\langle L^A LP_i, P_j \rangle = 0 \qquad i \neq j \tag{5}$$

where L^A is the adjoint of L (the transpose-conjugate matrix), the coefficients in Equation (4) are given by

$$\alpha_n = \frac{\langle E, LP_n \rangle}{||LP_n||^2} \tag{6}$$

The approach embodied in Equations (4) - (6) is known as the conjugate direction method [8]. Note that in the literature, this procedure is often presented for the special case where L is a symmetric and positive definite matrix. We make

no such restriction, and as a result the formulas presented here differ somewhat from those found, for instance, in [20].

The conjugate gradient method is a conjugate direction method which is augmented with a recursive procedure for generating the P-vectors according to (5). The P-vectors generated by the gradient algorithm, are, in fact, designed to represent the solution corresponding to a specific right-hand side E in (3). As a result, the solutions of most equations can be adequately represented by far less than the full set of N vectors [23]. This is an attractive feature of the conjugate gradient method over most other iterative techniques, providing that one is dealing with a single incident field.

The algorithm requires the user to provide J_o, an initial estimate of the unknown J. Normally, for well-conditioned systems, the choice of J_o has little effect on the number of iterations required for a solution, and a zero estimate is often used. However, it is important to note that the flexibility of accepting an initial estimate permits the user to terminate the iteration and start anew, using the current estimate of the solution as the initial estimate. This feature may be important when dealing with large-order equations in order to combat the round-off errors inevitably introduced due to the finite word-length of a computer.

A common form of the complete algorithm is given as follows [24] - [26]:

Initial steps

$$R_o = LJ_o - E \tag{7}$$

$$P_1 = -L^A R_o \tag{8}$$

Iterative steps $k = 1,2,\ldots$

$$\alpha_k = \frac{\langle E, LP_k \rangle}{||LP_k||^2} = \frac{||L^A R_{k-1}||^2}{||LP_k||^2} \tag{9}$$

$$J_k = J_{k-1} + \alpha_k P_k \tag{10}$$

$$R_k = LJ_k - E = R_{k-1} + \alpha_k LP_k \tag{11}$$

$$\beta_k = \frac{||L^A R_k||^2}{||L^A R_{k-1}||^2} \tag{12}$$

$$P_{k+1} = \beta_k P_k - L^A R_k \tag{13}$$

The residual norm

$$\frac{||R_k||}{||E||} = \frac{||LJ_k - E||}{||E||} \tag{14}$$

decreases monotonically as the algorithm progresses and is useful as an indication of the average error in the solution after k steps. The algorithm is usually terminated when the residual norm decreases to some prescribed value.

The conjugate gradient algorithm can be derived by considering the minimization of the quadratic functional [24], [25]

$$F(J_k) = ||R_k||^2 \tag{15}$$

Specifically, the P-functions are found by reducing the gradients of F at each estimate of J to an orthogonal set satisfying Equation (5). A set of such functions is said to be conjugate with respect to the operator $L^A L$, hence, the name "conjugate gradients."

In theory, the solution to an N-dimensional system will be found in at most N iterations. Even if no unique solution exists, the algorithm will converge in theory to the "minimum-norm" solution [22].

Based upon our own observations, a numerical solution accurate to several digits is found in N/3 iterations or less for most well-conditioned systems. The residual norm given by (14) would, for instance, quickly decrease from its initial value to something less than 1×10^{-4}. For poorly conditioned systems, the convergence is naturally slower and is exacerbated by round-off errors in any calculation involving the operator [22], [23]. Under these conditions, it is not uncommon for the residual norm to remain relatively constant for many iterations or even to grow under the influence of round-off errors. This situation arises occasionally in practice, and under such circumstances the algorithm may not converge. This is true in spite of the fact that, theoretically, the convergence of the gradient method is guaranteed in the absence of any machine error. There are numerous variations on the conjugate gradient method as it is presented here, some of which involve less computation and may be freer from the round-off problem [23]. This topic is currently under investigation by the authors.

It is often necessary in practice to analyze a single scatterer for many different sources of illumination. Equivalently, it is desirable to have an efficient means for solving Equation (3) for many different right-hand sides E. If Gaussian elimination is used to generate the inverse of a large matrix, any number of right-hand sides can be treated at an almost negligible additional cost. In theory, the conjugate gradient method could be adapted to test many sources efficiently by simultaneously expanding each solution in terms of the single set $\{P_i\}$. Unfortunately, complications arise which usually prevent this from being practical. As mentioned earlier, the P-vectors generated for a given E are specifically geared to represent one solution. For instance, in a case where the solution exhibited even-symmetry, all of the P-vectors generated to represent the solution were even-symmetric. Our experiences indicate that,

except in special cases, the entire set $\{P_i\}$, where the upper limit of i could be on the order of N for an N × N matrix, will be needed to treat several right-hand sides at one time. Because the conjugate gradient method uses a recursive algorithm to generate these functions, round-off errors progressively degrade their actual orthogonality. In practice, the severity of the round-off errors prevents the successful generation of the necessary vectors. For this reason, it appears that a nonrecursive algorithm for generating the P-vectors would be a better candidate for the treatment of multiple right-hand sides. Any practical method for treating large-order systems would do so without the need to store the P-vectors in computer memory. At this time, no approach satisfying these constraints is known to the authors, although they are currently experimenting with some algorithms that might be suitable for this purpose. Of course, until such a scheme is available, the conjugate gradient method may still be used to treat each right-hand side independently.

Certain integral equations suffer from "resonances" which occur when the equation permits homogeneous solutions, such as at frequencies where a scatterer is also a resonant cavity [27] - [29]. When this occurs, the operator is ill-conditioned, and the numerical solution is corrupted by the presence of the homogeneous solution and by round-off errors in the solution process. The conjugate gradient method can be useful as a flag to identify this situation, as the convergence of the method is significantly slower when the operator is poorly conditioned [23]. Methods for circumventing the difficulties arising in the "resonance" situation have been discussed elsewhere [27] - [29].

The above discussion is a brief introduction to the conjugate gradient method. Readers desiring additional information are encouraged to consult references [8], [10], [11], [20] - [26]. In the following section, several

scattering problems are presented as examples to illustrate the application of the method.

3. APPLICATIONS

The conjugate gradient algorithm can be applied directly to any discrete operator equation. The first step in a solution process is to select a discretization scheme and apply it to the integral equation. The method of moments is a general technique for converting continuous equations to matrix equations [5], and is used extensively in computational electromagnetics. However, the moment-method matrix equation for large-body scattering problems often exceeds the limits of computer memory and iterative methods which do not require the $N \times N$ matrix to be stored offer advantages. The first example to follow illustrates the conjugate gradient solution of a matrix equation with emphasis on minimal storage requirements.

Since the integral equations of interest are often convolutional in form, the Fast Fourier Transform (FFT) algorithm can in many cases be adapted to perform the convolution. Equations written as circular (periodic) or linear convolutions can be solved exactly using the FFT, and at a considerable savings over the comparable matrix multiplication. Examples of these situations are given below.

An alternate approach is to use the FFT as an approximation to the continuous Fourier transform, in order to compute convolution integrals which cannot be easily put into the form of discrete convolutions. This procedure is also discussed below.

Although these techniques can be applied to any size problem, we are primarily interested in geometries which are electrically too large to handle with conventional matrix methods. Comparisons between the execution times of the iterative methods and conventional matrix methods have been presented for small

geometries [15], [18]. To our knowledge, no systematic comparison has been published for large-order equations.

3.1. Solution of Matrix Equations

If the conjugate gradient algorithm is terminated after several digits of accuracy are obtained in the solution, it is often comparable to, and sometimes better in efficiency than, the Gaussian elimination solution of a single matrix equation [26]. In the elimination process, the N × N matrix is altered and must be stored in computer memory or in an out-of-core peripheral unit. This places an upper limit on the size of a scatterer which can be easily treated by matrix methods. The conjugate gradient method can be used to extend this limit, provided that the matrix elements are sufficiently redundant or can be generated from a relatively simple function subroutine. Each matrix element is needed twice per iteration; therefore, this approach will only be practical for large systems if the elements can be generated efficiently.

Several examples which were developed for conventional matrix solution and are well-suited for the iterative scheme include two-dimensional dielectric scatterers [30], [31], two-dimensional perfectly conducting scatterers [32], and three-dimensional dielectric bodies [33]. All of these are based on moment-method formulations using so-called pulse basis functions and point-matching, and all the matrix elements are closed-form expressions. For illustration, consider TM wave scattering by perfectly conducting two-dimensional cylinders, such as discussed by Harrington [32]. The matrix elements are given by

$$\ell_{mm} = 30\ \pi\ kd_n \left[1 - j\ \frac{2}{\pi}\ \ell n\ \frac{kd_n}{6.105}\right] \tag{16}$$

$$\ell_{mn} = 30\ \pi\ kd_n\ H_o^{(2)}\ (kR_{mn}) \tag{17}$$

where k is $2\pi/\lambda$, R_{mn} is the distance between the center of the mth and nth

subdivisions of the cylinder surface, d_n is the width of the n-th subdivision, and $H_o^{(2)}(\cdot)$ is the Hankel function of the second kind. In order to generate the matrix elements efficiently, the Hankel functions are interpolated from a look-up table. The size of the table is proportional to the maximum linear dimension of the scatterer, yet requires much less storage than the N × N matrix it replaces.

Results for the conducting cylinder example were obtained for problems involving 399 × 399 matrices. Matrix equations of this order are beyond the in-core storage capabilities of most modern computers. Figure 1 shows the magnitude of the surface current density on a square conducting cylinder at three frequencies. Similar results can be obtained for large dielectric cylinders that may, in general, be lossy and inhomogeneous. Figure 2 shows the polarization current induced inside a lossy dielectric cylinder consisting of over 500 cells [34]. We note that van den Berg has applied the conjugate gradient method to solve a similar problem involving 2500 cells in a dielectric cylinder [11], [12].

It is believed that the iterative method combined with the look-up table approach will permit many types of scattering problems to be solved for large geometries. The authors have used it for the examples discussed above, and found the efficiency satisfactory for large-order equations. In one case, an equation of order 1216 was solved on a Perkin-Elmer OS-32 computer [34]. However, not all integral equations can be reduced to matrix equations with simple elements; the complexity of the elements is usually directly proportional to the sophistication (and accuracy) of the discretization scheme used. As the complexity of each matrix element increases, the efficiency of the process decreases. Yet, even at its worst, the method offers an alternative to Gaussian elimination for the solution of large moment-method matrix equations.

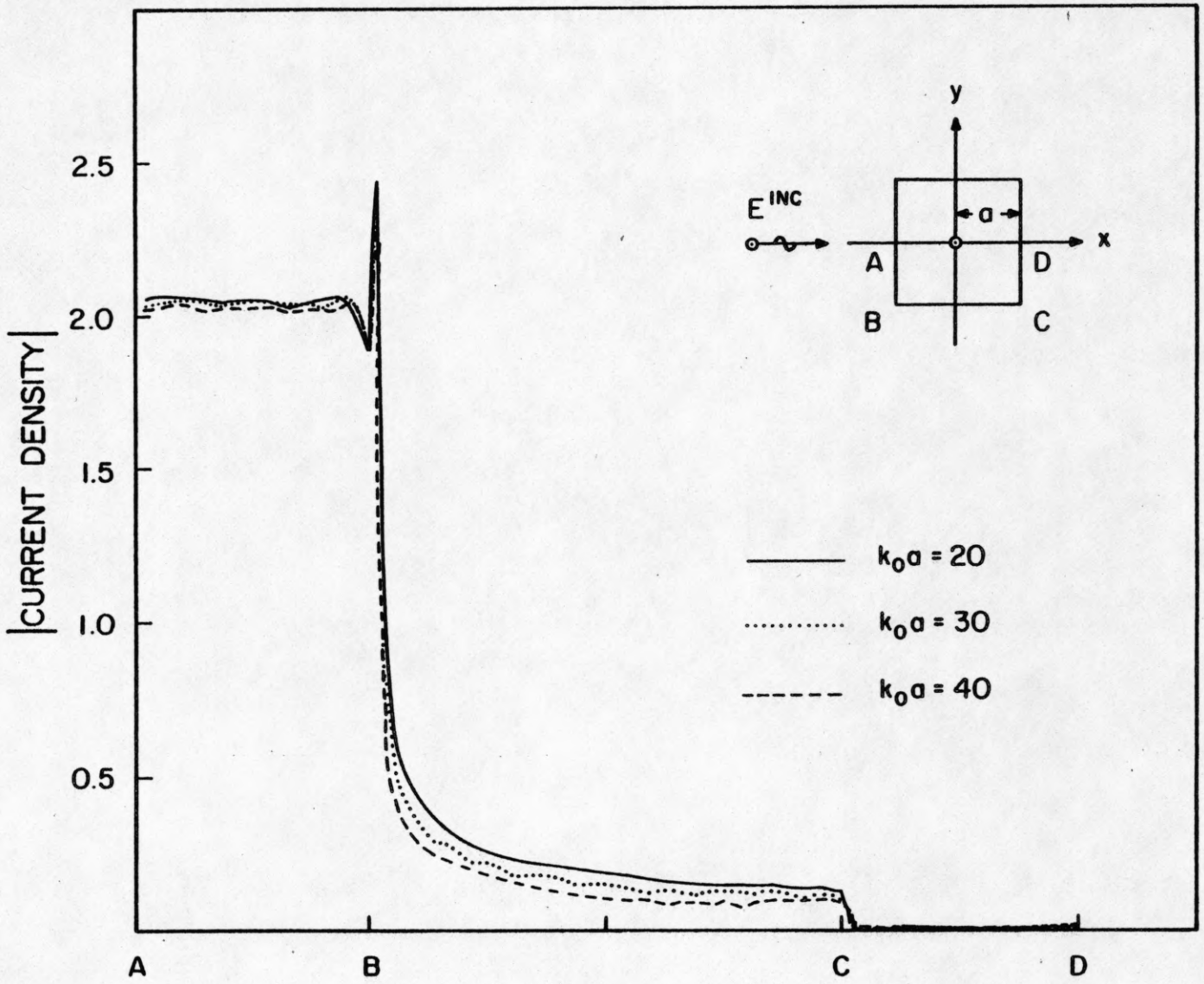


Figure 1. Magnitude of current density induced on a square cylinder at three frequencies. The cylinder model consisted of 339 cells.

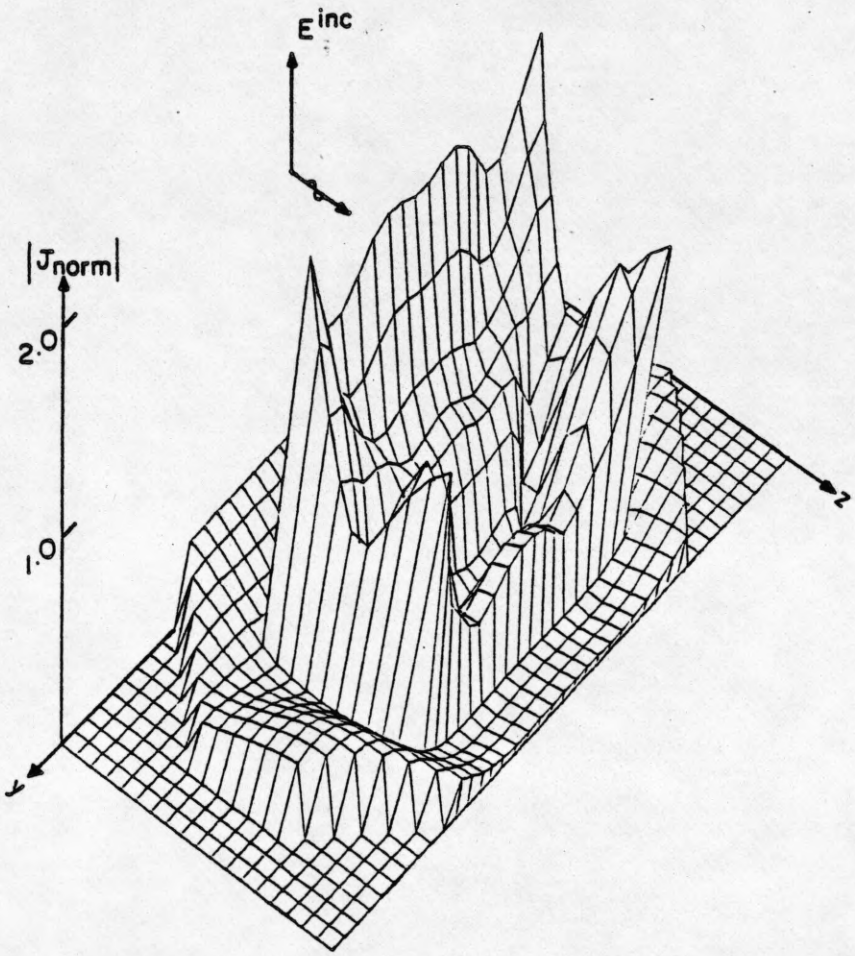


Figure 2. Polarization current induced inside a lossy dielectric cylinder. Central region has $\varepsilon_r = 51 - j31$, outer region has $\varepsilon_r = 5.6 - j1.1$. The current is normalized to the incident magnetic field.

3.2. Solution of Periodic Problems Using the FFT

An example of a problem well-suited for solution by the conjugate gradient method is the frequency-selective surface (FSS) shown in Figure 3. Frequency-selective meshes find many applications at optical and infrared wavelengths as band pass filters. The geometry is an infinite-periodic extension of a single rectangular cell, and for plane-wave scattering an integral equation for the vector components of the current on the metallic portion of the cell can be derived using Floquet's theorem [35]. The entire rectangular cell can be discretized via the moment method to yield a vector equation containing scalar components of the form

$$E_{ij} = \sum_{m=1}^{M} \sum_{n=1}^{N} J_{mn} K_{i-m,j-n} \tag{18}$$

Equation (18), written in the space domain, represents a circular discrete convolution. The K_{pq} of Equation (18) are actually each a double-infinite summation over the Floquet modes. Equation (18) can be written in the discrete Fourier transform domain as

$$\tilde{E}_{\alpha\beta} = \tilde{J}_{\alpha\beta} \tilde{K}_{\alpha\beta} \tag{19}$$

It may be undesirable to compute $\tilde{K}_{\alpha\beta}$ by applying the FFT to the K_{ij}, and as an alternative, the $\tilde{K}_{\alpha\beta}$ can be approximated by samples of the continuous Fourier transform of K, which is usually a simple analytic expression (not a summation) [36]. This suggests that a significant savings in computation can be realized by operating in the spectral domain. This entails using the FFT to transform J_{nm} to $\tilde{J}_{\alpha\beta}$, performing the multiplication indicated in equation (19), and using the inverse FFT to find E_{ij} from $\tilde{E}_{\alpha\beta}$. This approach is often used for problems involving periodic geometries [37], [38].

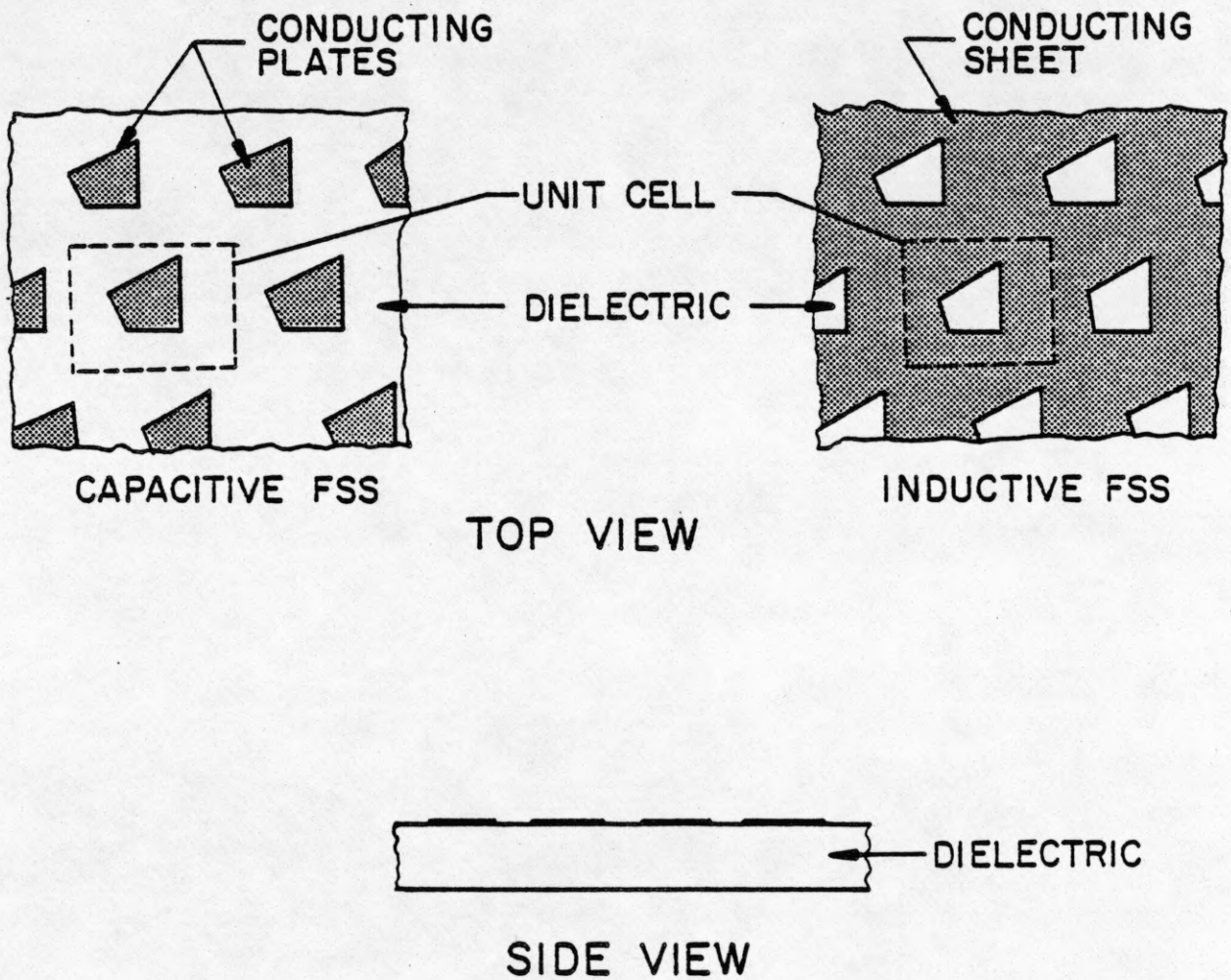


Figure 3. Frequency selective surface.

This type of problem is ideally suited for solution by the conjugate gradient method because of the low storage requirements imposed by the $\tilde{K}_{\alpha\beta}$ and the efficiency of the FFT algorithm. The approach permits a wide range of choices of basis and testing functions in a moment-method formulation as long as the discretization of the rectangular cell is evenly spaced in both dimensions. However, whereas a conventional moment-method approach is limited by the size matrix that must be stored, the conjugate gradient method permits the treatment of much larger problems. Recently, the conjugate gradient method was used to analyze an FSS with over 4000 unknowns [17].

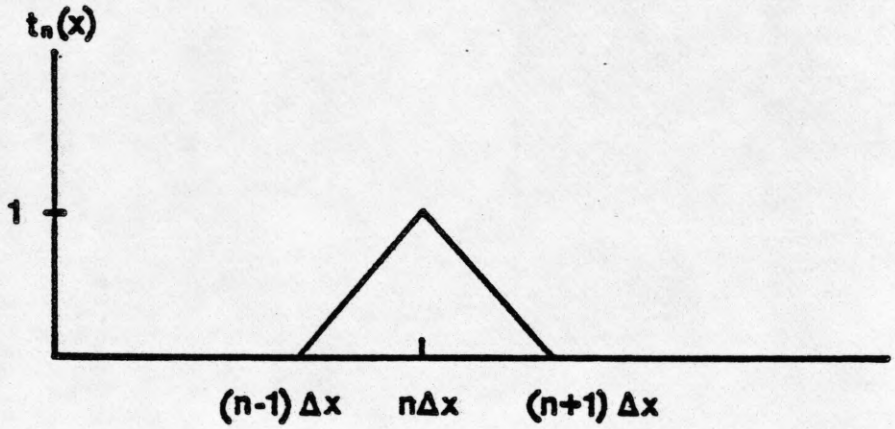
3.3. Problems Which Are Linear Discrete Convolutions

The previous example discussed the use of the conjugate gradient method for periodic geometries. The circular discrete convolutions that arise can be performed efficiently using the FFT. Certain nonperiodic geometries can be discretized in such a way that the associated equations become linear discrete convolutions, and these can also be computed with the FFT. In the latter case, "zero-padding" must be incorporated into the algorithm [39]. Examples of problems well-suited to this approach are planar structures and two- and three-dimensional dielectric bodies.

As an illustration, consider TE-wave scattering by an imperfectly conducting, or resistively coated planar strip. Following Ray and Mittra [18], the discretized integral equation can be written as

$$E_m = R_m J_m - \sum_{n=(1-N)}^{N-1} J_n G_{m-n} \qquad (20)$$

for the choice of basis functions pictured in Figure 4. R_m is the resistance of the m-th strip as defined by Senior [40]. Since (20) contains a discrete convolution, the FFT can be incorporated into a conjugate gradient algorithm to provide an efficient solution. Ray and Mittra [18] have shown that, in addition



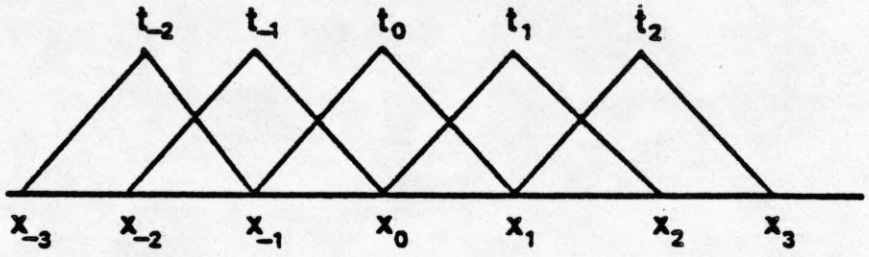


Figure 4. Relative position of the basis functions on the strip.

to a savings in storage, the conjugate gradient method achieves a savings in computation time as compared to the Gaussian elimination solution of Equation (20) [18].

An example of the results for one strip configuration is pictured in Figure 5, following Ray and Mittra [18]. The three-dimensional problem of scattering from resistive plates has been analyzed using a technique analogous to that presented for the resistive strip, and in particular, used for plate sizes requiring over 3000 unknowns [18], [19].

3.4. Use of the FFT in More General Problems

The above examples illustrate several ways in which the conjugate gradient method can be incorporated into the solution process for large scattering problems. In every case, the moment-method formulation is adhered to and extended to treat larger geometries. However, the above examples all suffer from some limitation. The most general approach is the matrix solution, yet it may only be practical if the matrix elements are relatively simple. The FFT-based approaches discussed above are superb for certain restricted geometries, but aside from planar structures and finite circular cylinders, the only nonperiodic scatterers which can be treated are penetrable dielectric bodies. The limitation is due to the discretization process itself; in all the cases discussed above, the conjugate gradient algorithm was used to solve a numerical system resulting from an application of the method of moments to the original problem. The moment method technique is well-understood and very systematic; however, other discretization schemes may be better suited for use with the FFT.

An alternative approach to solving scattering problems is based upon a procedure known primarily by the name "Spectral Iterative Technique" [17], [18], [34], [37], [41], [42]. To distinguish this technique, which involves using the

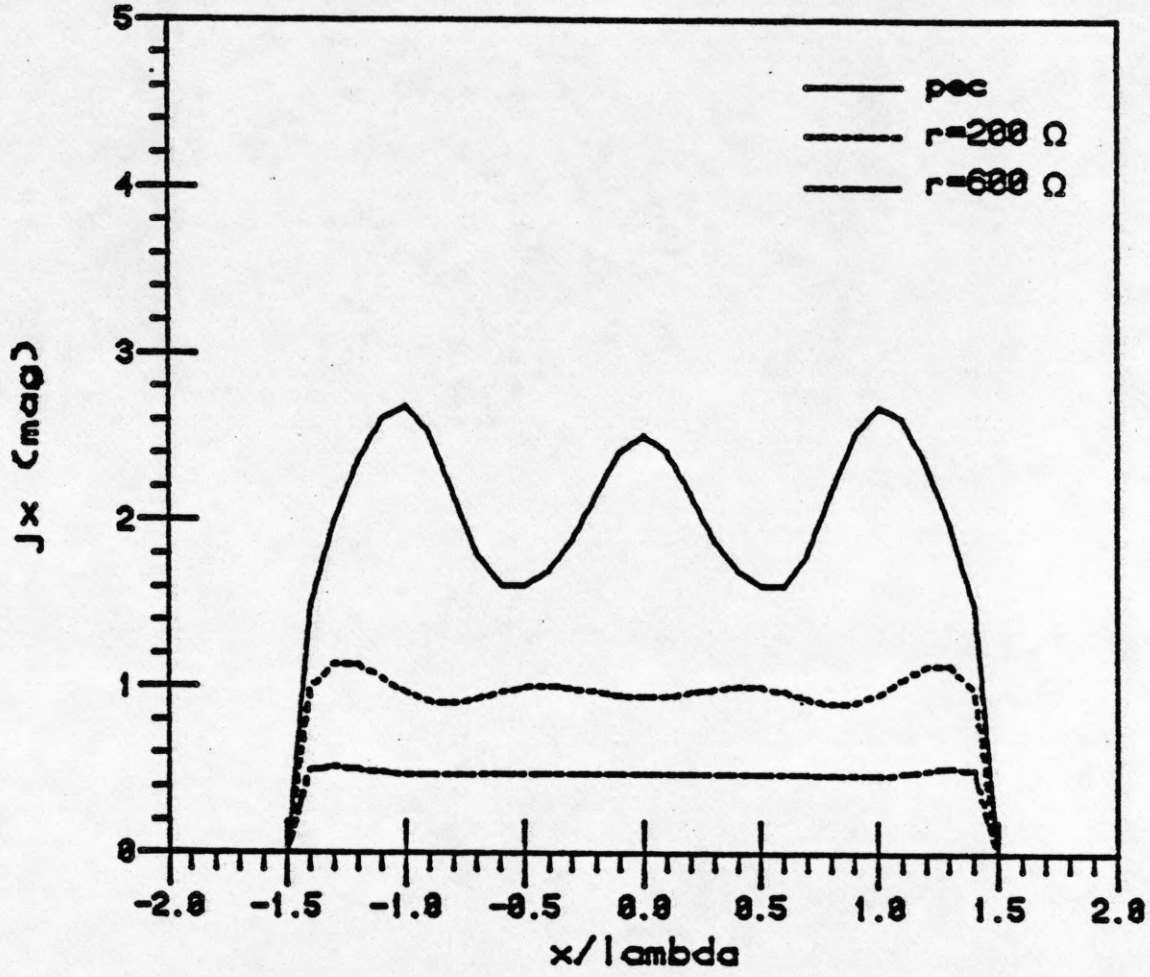


Figure 5. Magnitude of the induced current on a strip for several values of the constant surface resistance.

strip width = $3\lambda_o$
TE polarization
normal incidence

FFT in an iterative procedure, from the techniques discussed above using the FFT with the conjugate gradient method, we introduce the title "Spectral Iterative" (SI) to those approaches where a continuous convolution integral is approximated using the FFT. In the previous examples, the FFT was used to perform discrete convolutions. In the SI approach, the quantities of interest are sampled over a regular grid of points. This sampling scheme is distinctly different from the moment-method discretization scheme, and thus should be considered a separate method. The conjugate gradient approach discussed in the examples given above is really nothing more than a way to apply the moment method to larger problems. The conjugate gradient iterative procedure may also be used as an SI technique, in which the moment method formulation is avoided in favor of a sampling discretization that anticipates the use of the FFT. The SI approach was used in the past with an algorithm based upon an iteration procedure that did not guarantee convergence. The conjugate gradient SI method does ensure convergence, and thus permits the SI technique to be applied to many additional scattering problems.

For instance, van den Berg and De Hoop have used the conjugate gradient method to analyze scattering from a rough interface [13]. Their approach incorporated an FFT approximation to a Fourier transform integral, and thus is an SI technique. The SI approach offers a general method for the treatment of large-body scatterers, as it appears to have few fundamental limitations as to the types of problems that can be treated with the FFT. Future work in this area will produce a systematic way of using the method and analyzing the accuracy of the results.

4. DISCUSSION

We have presented the conjugate gradient algorithm and discussed some of its features. Many of the remarks on the attributes and limitations of the method are based upon our own observations made when using the method to solve pertinent integral equations. In some cases, our observations may not concur with the recommendations of others; for instance, it has been suggested that the conjugate gradient method is useful for the solution of very ill-conditioned equations [10] and that it is suited for handling multiple incident fields. However, our findings seem to be at odds with these suggestions. As the method has only recently been applied to problems in electromagnetic scattering, it is expected that the future will provide additional clarification.

The advantages of the conjugate gradient method for the solution of large scattering problems lie primarily in the fact that in many cases no alternatives exist aside from a brute-force Gaussian elimination solution of the moment-method matrix using out-of-core storage. For many equations, the conjugate gradient method permits the solution of large problems without a corresponding need for large blocks of computer memory. The conjugate gradient method may not be the best choice in a given situation; it should be considered an alternative which may or may not be useful depending on the problem. Needless to say, much work remains in the extension of this technique to general scattering problems.

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