CROSS-TYPE ALGORITHM FOR EFFICIENT SOLUTION OF ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS IN TWO DIMENSIONS

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ABSTRACT

In the work reported here a computationally efficient algorithm for the solution of elliptic partial differential equations on rectangular domains is given. The algorithm reduces the solution of the problem to the solution of a series of one dimensional problems and thus the resulting system of linear equations may be solved with relative ease as demonstrated by an example. (key words: numerical solution, partial differential equations)

INTRODUCTION

The solution of steady-state problems of heat conduction and electrostatics in two dimensions often involve the solution of the partial differential equation

$$\nabla \cdot [g\nabla V] - Q(x,y) \tag{1}$$

where V(x,y) is the scalar field variable and Q(x,y) represents a source term. The parameter g a property of the medium. In the thermal conduction problem it is the thermal conductivity and in the electrostatic problem it is the dielectric constant. If the medium is isotropic the equation reduces to the well-known Poisson equation

$$g \nabla^2 V - Q(x,y) \tag{2}$$

In the work discussed here a new, strongly implicit method for the solution of elliptic partial differential equations such as (1) and (2) will be presented. The numerical solution of such problems using the finite difference representation of the partial derivatives results in a problem of the repeated solution of a set of linear equations in matrix form.

$$A X - Y \tag{3}$$

where A is an $n \times n$ square matrix, X is a unknown n-vector and Y is a known n-vector on the right side of the equation.

FUNDAMENTALS OF THE ALGORITHM

Using a strongly implicit approach for a solution of matrix equation (3) the following formula is proposed.

$$X - X + A_a^{-1} (Y - A X)$$
 (4)

The above formula can be used in an iterative procedure for finding unknown vector X using it in the form

$$X_n = X_p + A_a^{-1} (Y - A X_p)$$
 (5)

where X_p and X_n are respectively previous and new values of the unknown vector X during the iteration procedure. It can be easily shown that the process will converge if the eigenvalues of $I - A_a^{-1} A$ are interior to the unit circle.

The matrix A_a is an approximation to the matrix A. The matrix A_a is chosen in such way that it can be easily inverted. In equation (5) inversion of matrix A_a is equivalent to of finding an approximate solution and this is a key issue of this presentation.

FINDING AN APPROXIMATE SOLUTION

In order to describe this approach let us consider the rectangular shape shown in Fig. 1-a. The algorithm proceeds as follows:

1. The Poisson equation is solved for two quasi one-dimensional cases between points A and B, and between points C and D. During the quasi one-dimensional solution only some fraction of the sources at each node is used, namely $Q_{j,i} = \alpha_{j,i} Q_{j,i}$, where $\alpha_{j,i}$ for horizontal computation is

$$\alpha_{j,i}^{h} - \frac{g_{j}^{h} + g_{j+1}^{h}}{g_{j}^{h} + g_{i}^{\nu} + g_{j+1}^{h} + g_{i+1}^{\nu}}$$
 (6)

$$\alpha_{j,i}^{\nu} = \frac{g_{i}^{\nu} + g_{i+1}^{\nu}}{g_{j}^{h} + g_{i}^{\nu} + g_{j+1}^{h} + g_{i+1}^{\nu}}$$
(7)

Note also that $\alpha_{j,i}^{\ h} + \alpha_{j,i}^{\ v} = 1$. In the case for isotropic media and equal mesh size in both directions the $\alpha_{j,i}$ are both one half. The coefficients of equations (6) and (7) are defined in Figure 1-b. The derivation of above formulas is too complex to include in this summary.

- 2. As a result most likely at center point E (see Fig. 1-a) two different values of the scalar field variable V are obtained and the resultant value is computed as an average of these two values.
- 3. Using the value of the scalar field variable V obtained above at point E the quasi one dimensional solution of the differential equation for all four branches can be obtained.
- 4. As a next step each of four subrectangles are divided by the crosses on the smaller rectangle as shown in Fig. 1-a with the points *F*,*G*,*H*,*I* where potentials are known. The procedure described above is repeated for those smaller rectangles.
- 5. In the following steps the subrectangles are bisected again and process is repeated until the size of subrectangles is small enough to satisfy the resolution requirements.

One can note that in this procedure the analyzed structure will always be divided such that the number of meshes are equal to a power of two. This is a minor limitation of this algorithm because the mesh need not be regular and the medium need not be homogenous or isotropic.

COMPUTATIONAL RESULTS

The method is very similar to the method used by Stone [3] but in most cases it converges more rapidly than the Stone algorithm. This is because in the Stone method errors in one direction are usually eliminated very rapidly and in the second direction convergence is much slower. Therefore, frequently in the Stone algorithm every second iteration the main direction is changed. The algorithm described here with cross type computation converges very rapidly in both directions.

It requires only 5 to 8 iteration to obtain sufficient accuracy, it is slightly faster than the Stone algorithm and of course it is much more efficient than the commonly used Successive OverRelexation (SOR) algorithm [7] which requires a few hundred iteration steps in order to obtain the same accuracy. As an example of the application consider the solution of the Poisson equation on the square domain with a uniform source near one corner. The medium will be assumed to be homogeneous and isotropic with zero boundary conditions along the edges of the square. Computations were done with equal mesh size in both directions and grid size of 32×32 meshes. Figure 2 shows the scalar field variable distributions obtained in the example for the first six iteration steps. Figure 3 presents the microscale errors e_{ji} defined by equation (8) which would eventually be identically zero at each node for a pure fine difference approach.

$$e_{j,i} = \frac{V_{j-1,i} g_j^h + V_{j+1,i} g_{j+1}^h + V_{j,i-1} g_i^{\nu} + V_{j,i+1} g_{i+1}^{\nu} - Q_{j,i}}{g_i^h + g_i^{\nu} + g_{i+1}^h + g_{i+1}^{\nu}} - V_{j,i}$$
(8)

One can notice in Fig. 3 that an error is distributed along cross arms and with a few iterations practically disappears. In the example presented for the purpose of demonstration the distribution used was very simple and regular. If any different source distribution with very complicated were used shape the convergence was equally rapid.

CONCLUSION

The method presented here is very efficient for homogenous materials and it seems to be very suitable for solution of the Poisson equation for the numerical analysis of semiconductor devices. The method was also tested for cases with nonhomogeneous materials where it was assumed that medium property g differed by two orders of magnitude. In these cases number of required iteration steps increased by an order of magnitude.

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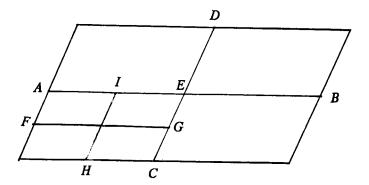


Fig. 1.a Illustration of cross-type algorithm

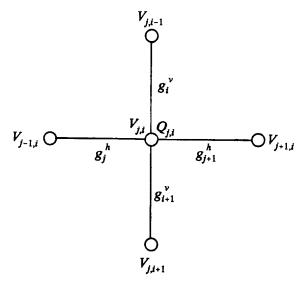


Fig. 1.b. Single node of computation grid

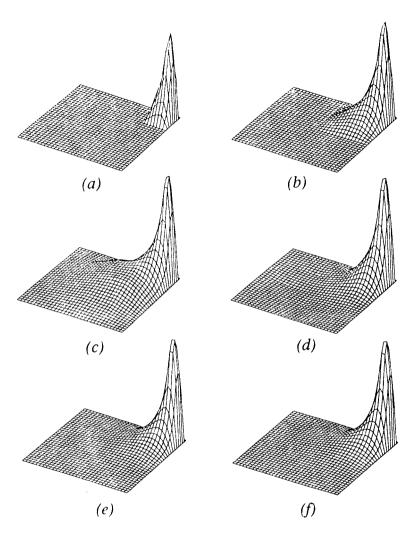


Fig. 2. Scalar field distribution obtained for the first six iteration steps

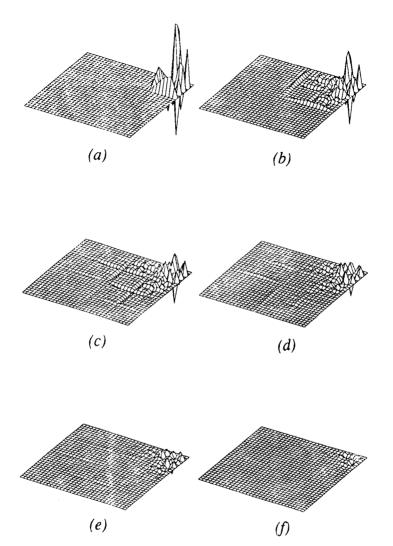


Fig. 3. Microscale errors defined by equation (8) for the first six iteration steps.

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