SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 3
Edited by G. Baccarani, M. Rudan - Bologna (Italy) September 26-28, 1988 - Tecnoprint

A Multigrid Approach to Solving Poisson's Equation for a p-n Diode

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August 17, 1988

1 Introduction

The solution of the Poisson equation, using the finite element method, offers a multitude of decisions regarding the solution procedure. Factors which will influence these decisions include both the ease of implementation and the computer time required. Multigrid is an approach to the solution method. In this paper, the use of multigrid with the very straightforward Jacobi relaxation is described. Alone, Jacobi relaxation is slow to converge. However, problems associated with it are addressed by multigrid, and a neat and useful algorithm results.

It this paper, the ideas of multigrid are summarised. These ideas are extended to cover the use of linear interpolation with the non-linear Poisson equation. The paper concludes with a two-dimensional example, illustrating the algorithms developed.

2 The idea behind Multigrid

The essential idea of multigrid is that, for accuracy, a fine mesh is required for solving a partial differential equation. This is in order to resolve local detail in the solution. However, often much of the computational work is required to establish the more long-range features of the solution, which would be attained more accurately on a coarser grid. Thus an efficient solution technique would allow solution of the long range features, or low frequency components, on a coarse grid whilst the high frequency components are improved on a companion fine grid. The concept of different frequency components of solution leads to a natural analysis of the problem in the frequency domain by Fourier analysis of the deviation from solution and the updates.

The concept of solution on 'companion' coarse and fine grids gives rise to a hierarchy of grids (multigrid) with a solution strategy exemplified by the two grid scheme below.

Start with an approximate solution on the fine grid. (We shall return to this in a later section)

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- Smooth the error on the fine grid, to reduce the high frequency terms in the Fourier expansion.
- Solve for the low frequencies on the coarse grid.
- Transfer the information from the coarse grid back to the fine grid solution.
- Smooth again on the fine grid, to reduce high frequency terms.
- Converged? If not, repeat the process.

Finish with a solution of the required accuracy on the fine grid.

Note that this extends directly to more than 2 grids. The use of more than two grids gives rise to the name "multigrid".

Such a scheme requires the definition of appropriate mappings:

Firstly, the smoothing operator. This will also require an idea of how much smoothing to perform.

Secondly, the contraction map, which transfers information from the fine to the coarse grid. This should include definition of the equations to be solved on the coarse grid, where it is essential that the coarse grid equations are exactly satisfied when the exact solution on the fine grid is transfered.

Thirdly, the prolongation or extension map, which is required to transfer coarse grid information back to the fine mesh.

In addition, an initialisation procedure is required which provides a suitable initial guess on the fine mesh.

Multigrid has been used for a variety of linear problems. However, the Poisson equation is non-linear and this presents challenges for multigrid. In this paper, a particular choice of mappings is presented. This combination is used to solve a practical 2-dimensional problem, showing that the multigrid philosophies can be successfully extended to the non-linear Poisson equation.

3 The Multigrid Mappings

3.1 Definition of the Meshes

The meshes used to develop this multigrid scheme use right-triangular elements. The coarse grid is uniform, and the fine grid is created by equally splitting each of these triangles into four smaller triangles. In the following analysis, a uniform mesh of characteristic mesh size h_k is used. This definition of the mesh ensures that the coarse mesh nodes are a subset of the fine mesh nodes. This is a simple but not necessary restriction.

Linear shape and weight functions are used. The shape function associated with node j is denoted by N_j. A superscript f or c denotes the fine or coarse grid shape function respectively. Similarly, R_j with a superscript f or c denotes the residual at node j on the fine or coarse mesh respectively.

3.2 The Smoothing Operator

The purpose of the smoothing operator is to reduce the high frequency components in the error. Relaxation has been used for this purpose, Hackbush (1981), in particular both Gauss Seidel and Jacobi relaxation. Current trends in computation are towards parallel architectures. Moreover, the use of Gauss Seidel relaxation is dependent upon the ordering of the nodal equations. This suggested that Jacobi relaxation, if sufficient, would be simpler.

The amount of smoothing to perform is addressed later in the paper.

3.3 The Contraction Map

The contraction map is required to transfer information from the fine grid to the coarse grid. Our goal is to gain the overall picture of the fine mesh solution, using the coarse grid. The fine mesh equations are multiplied by the coarse mesh weight functions. A Galerkin weight is used, so the weight function is the same as the shape function. The weighted residual statement is

$$R_j^c = \int_\Omega \nabla N_j^c \sum_{i=1}^{n^f} \nabla N_i^f \psi_i^f .d\Omega + \int_\Omega N_j^c \rho^f(\psi).d\Omega$$

The coarse mesh shape function can be expanded as a weighted sum of the fine mesh shape functions. For linear shape functions, this linear sum is

$$N_j^c = \sum_{k=1}^{n^f} N_k^f .N_j^c(k)$$

where $N_j^c(k)$ denotes the value of the coarse mesh shape function at node k of the fine mesh. The sum can be substituted into the first equation. Rearranging the result shows

$$R_j^c = -\sum_{k=1}^{n^f} N_j^c(k).\left(\sum_{i=1}^{n^f} \int_\Omega \nabla N_i^f .\nabla N_k^f \psi_i^f .d\Omega + \int_\Omega N_k^f .\rho^f(\psi)d\Omega\right)$$

The second sum in this equation is precisely the node k residual on the fine mesh, so

$$R_j^c = \sum_{k=1}^{n^f} N_j^c(k).R_k^f$$

Showing the coarse mesh residual to be a weighted linear sum of the fine mesh residuals. Denote this map from the fine grid to the coarse grid by I_f^c.

3.4 The Equations On the Coarse Grid

One problem with multigrid is determining the consistency of the solution method. For instance, suppose that the fine mesh solution has converged. Then the coarse grid update should be zero. Generally, the coarse grid update should take the current approximate solution closer to the actual solution.

Brandt (1982) tackles this problem via the Full Approximation Scheme (FAS). For completeness, this is summarised.

Let the system of equations be denoted by Lu=f. Then Brandt shows the coarse grid equations to be

$$L^c \hat{u}^c = f^c$$

where $\hat{u}^c$ approximates the full solution on the coarse grid. Now let $\bar{u}^f$ denote the approximate solution on the fine grid. Brandt shows that

$$f^c = I_f^c R^f + L^c(\hat{I}_f^c \bar{u}^f)$$

Here, I_f^c denotes the mapping of the residuals from the fine to the coarse mesh, whilst $\hat{I}_f^c$ denotes the mapping of the solution vector from the fine to the coarse mesh.

3.5 The Amount of Damping and Smoothing

To prevent oscillations when smoothing pointwise by a Jacobi scheme, some degree of damping is required. For the linear laplace equation, the optimal damping for high frequency componenets can be shown to be 1/2.

A technique called local mode analysis may be used to determine the optimal relaxation parameter. This is fully described by Hackbush (1981).

Liddiard (1986) shows that for the Poisson equation, the optimal damping parameter, α, is given by

$$\alpha = \left| \frac{1}{2 - \frac{h_k^4}{4}(p+n)} \right|$$

The corresponding amount of smoothing may be calculated. If the range of frequencies to smooth is denoted by (θ_1, θ_2) the smoothing parameter μ is given by

$$\mu = \left| w \left[\frac{cos(\theta_1) + cos(\theta_2) - 2}{2} + \frac{h_k^4}{4}(p+n) \right] + 1 \right|$$

For each iteration, let $\bar{\mu}$ be the maximum value of μ. Then the sequence of values $\bar{\mu}$ indicates the amount of smoothing to be performed. In order to decrease oscillations by an order of magnitude (a rule-of-thumb), the product of successive values of $\bar{\mu}$ should be less than 0.1. The multigrid code can monitor this product, and perform the required amount of smoothing accordingly. Typically, the example shown in this paper uses 3 smoothing sweeps.

3.6 Initialisation of the Fine Grid Solution

A very practical problem is the initialisation of the solution on the fine grid. One easy way is to simply interpolate a coarse grid solution. The advantage of this is the relatively inexpensive solution on the coarse grid, the disadvantage is that the interpolation is inaccurate and not very effective. Such a method may be improved.

The nodes in the coarse grid have already reached a coarse grid solution. These nodes are therefore likely to be more accurate than the extra (interpolated) nodes of the fine grid. If the accurate nodes are held constant, it should be relatively inexpensive to improve the extra nodes. Such improvement may be done using the smoothing algorithm, giving a variation of the red-black Jacobi schemes. However, these new nodes are connected, and a large number of sweeps are required to reach equilibrium. Typically, three sweeps are sufficient to capture the essence of the solution without excessive computation.

4 Results

The example is a p-n junction. The first model shows one-dimensional behaviour. The diode is abrupt, equidoped at 10^{16} per cubic centimetre. It is shown in Fig 1, with the two meshes in Fig 2. Contour plots of the potential are shown in Fig 3.

The effectiveness of the smoothing alogorithm is seen by examining the residuals. Fig 4 shows these before and after three relaxation sweeps. The contours are at 0.5 units and 0.1 units, respectively. Counting the contours illustrates the accuracy of the smoothing algorithm analysis.

The second diode show two-dimensional behaviour. This is again abrupt, equidoped at 10^{16} per cubic centimetre. The example, meshes and resulting contour plot are shown in Figs 5,6 and 7.

5 Extensions to This Work

The scheme may be directly generalised to more grids. The general form of the contraction map also allows for the definition of non-nested grids. This offers very exciting prospects for adaptive meshing schemes. Questions to address include the pattern of movement between more than two grids, commonly known as v or w cycles. Other extensions include addressing the continuity equations, and investigating the effectiveness of more involved interpolation schemes.

Standard multigrid techniques, such as tor-extrapolation, may be used to improve the efficiency of the method.

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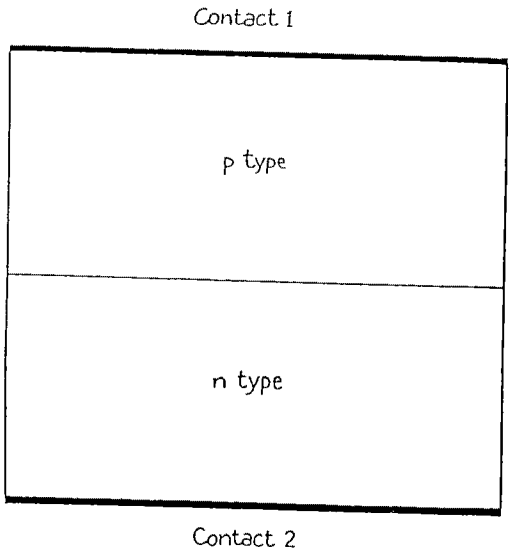


Fig 1

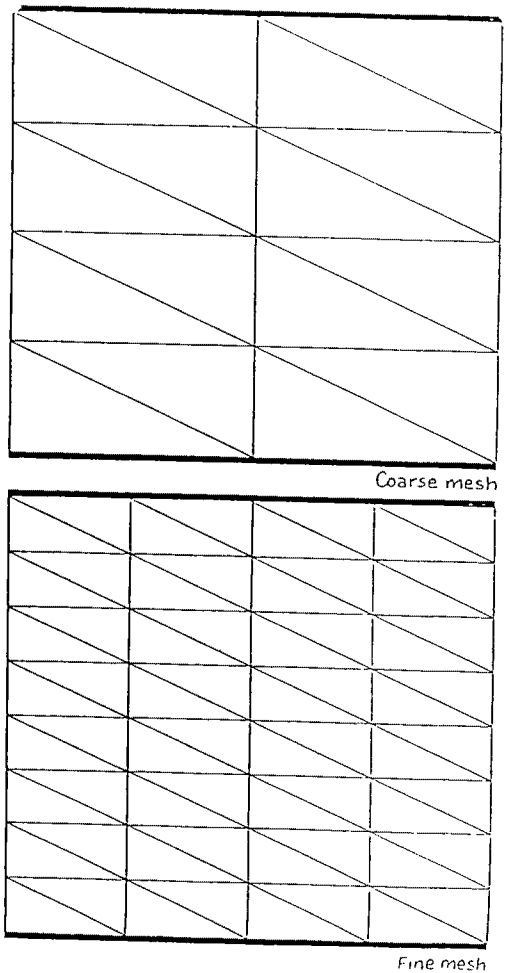
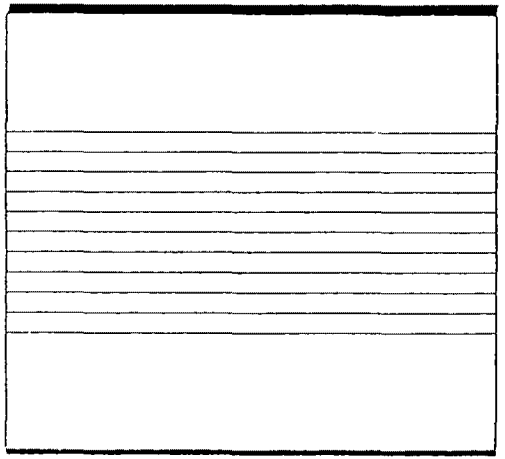


Fig 2.


Coarse mesh

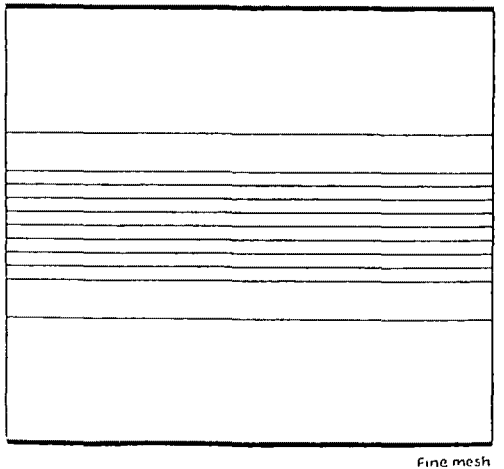
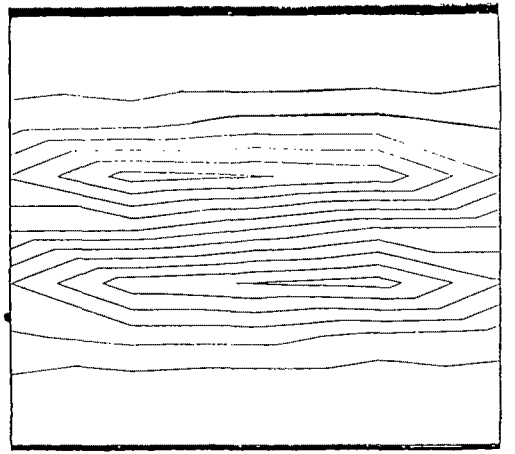

Fine mesh

Fig3


'A'- before Smoothing

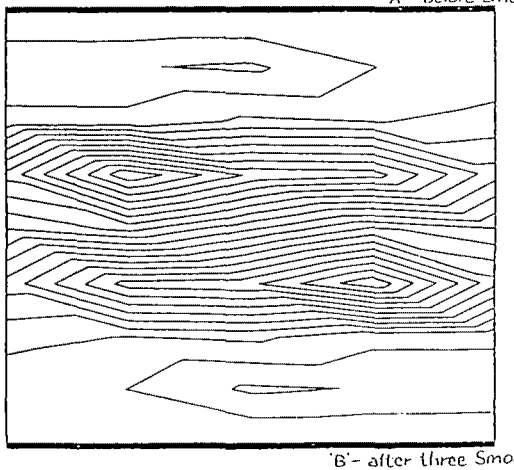
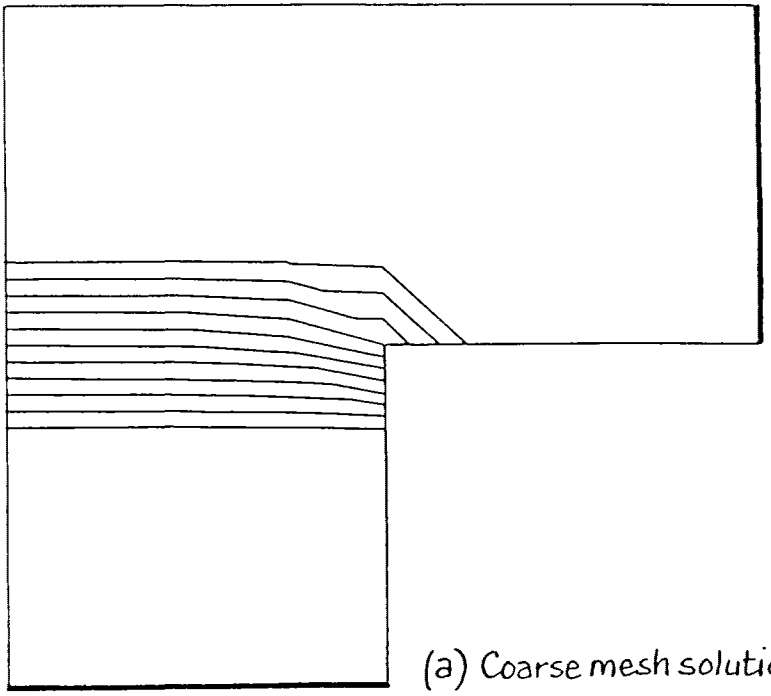

'B'- after three Smoothings

Fig4.

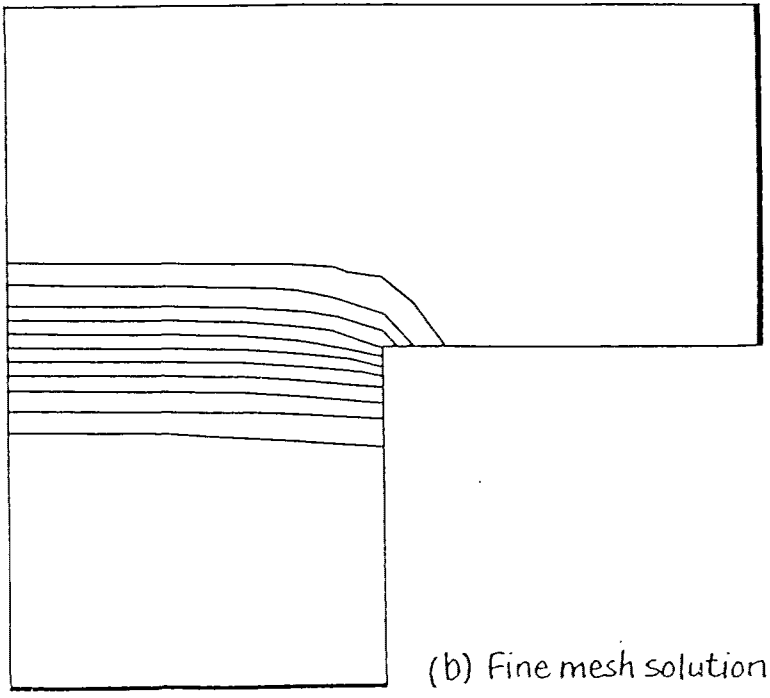
Mesh for test problem

Fig 6

Fig 5



(a) Coarse mesh solution



(b) Fine mesh solution

Fig 7