AUTOMATIC GRID CONTROL IN DEVICE SIMULATION

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SUMMARY

Automatic grid control for finite differences meshes is a difficult task because only very few mathematically founded criteria for adaptive grid refinement can be given which may be implemented in a computer program with reasonable effort. Especially for the solution of the semiconductor equations, a coupled system of nonlinear partial differential equations, most strategies for fully automatic both time and space grid control are heuristic or based on physical considerations.

We present some criteria for the construction of initial space grids, for adaptive space grid refinement and fully automatic time step control which are implemented in our two-dimensional transient device simulation program BAMBI.

1. INTRODUCTION

For the numerical solution of partial differential equations fully self-adaptive grids are well suited to optimize the ratio between the number of unknowns and the accuracy of the solution. In device simulation a time dependent coupled system of three nonlinear partial differential equations has to be solved:

$$\text{div grad } \psi = \frac{q}{\epsilon} \cdot (n - p - C) \qquad (1) \text{ Poisson equation}$$

$$\text{div } \vec{J}_n - q \cdot \frac{\partial n}{\partial t} = q \cdot R \qquad (2) \text{ Continuity equation for electrons}$$

$$\text{div } \vec{J}_p + q \cdot \frac{\partial p}{\partial t} = -q \cdot R \qquad (3) \text{ Continuity equation for holes}$$

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where ψ, n, p denote the three independent unknown functions for the electrostatic potential and the concentrations of electrons and holes, respectively. $\vec{J}_{n,p}$ denotes the current densities for electron and hole current. q is the elementary charge, ϵ stands for the absolute permittivity of the semiconductor material, C for the net doping concentration, R denotes the net generation/recombination. Further information about this problem can be found in [1].

For the discrete formulation of (1)–(3) the Scharfetter-Gummel approach has been choosen in many programs. This formulation can be found thoroughly discussed in [1]. In [2] some basic ideas about grid design in process and device simulation have been presented. We discuss some strategies in detail for fully self-adaptive both time and space grid control in device simulation. They are illustrated by examples which have been computed with our two-dimensional transient device simulator BAMBI [3]. The solution is computed on a generalized finite differences grid, a so called 'Finite Boxes' grid.

2. SELF–ADAPTIVE SPACE GRID

2.1. Initial Space Grid

The design of an initial space grid is a very important task since the number of grid points required in the adaptive process and the convergence behaviour are very sensitive to the construction of a start grid. Usually it is based on an analysis of the doping profile C. A popular strategy is the evaluation of the gradients of the doping profile in order to resolve p-n junctions in a proper way. However, this strategy fails, if abrupt junctions occur or if a constant doping is assumed (e.g. MESFET's). In the latter case additional information is often given by the geometry of the device: At points with a change of the boundary conditions a singularity in the electric field has to be regarded (e.g. change from a contact (Dirichlet) to a Neumann boundary, origin of a cylindrically symmetric coordinate system, reentrant corners). By using this information to define the initial grid difficulties for start meshes which do not account for singular points can be avoided. Therefore we introduce new grid points near these singular points.

In Fig. 1 a,b the geometry and the meshes of final accuracy of a simple resistor with a constant doping (potential problem) can be seen. In (a) the knowledge of the singularity was not taken into account, while in (b) three lines close to the singularity have been introduced. It should be mentioned that all other lines result from criteria for the regularity and for the quasi-uniformity of the grid.

2.2. Self–Adaptive Space Grid

Fully self-adaptive space grid control is usually based on the equidistribution of a suitably choosen function over the integration domain [4]. In device simulation the local discretization error of the Poisson equation

$$\text{div grad } \psi = \frac{\rho}{\epsilon} = \frac{q}{\epsilon} \cdot (n - p - C) \qquad (4)$$

is considered where ρ denotes the space charge. Mathematical tools fail in treating the whole system or the numerical effort will be too great.

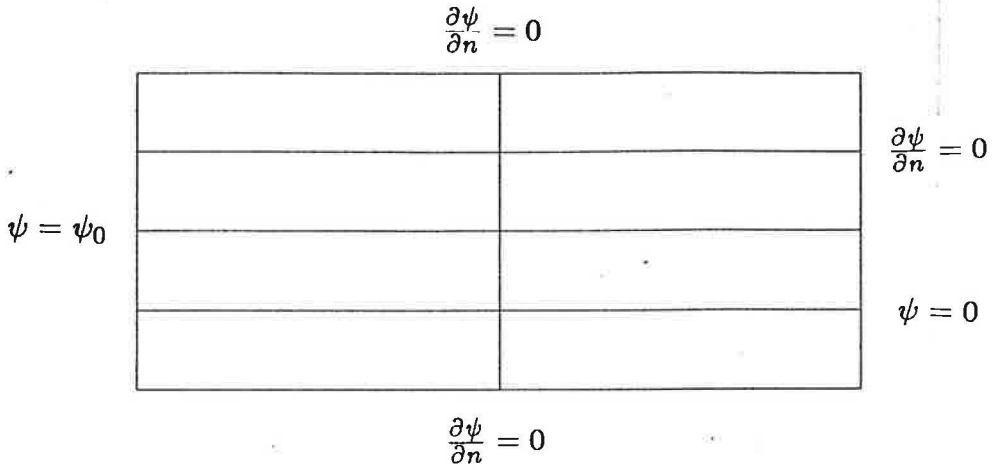

Fig. 1a Geometry and mesh of a resistor without knowledge of singularity

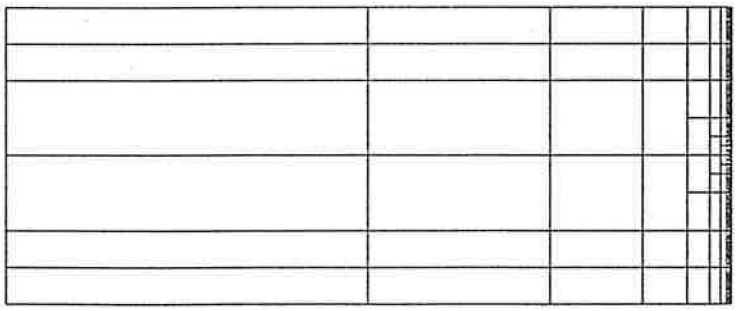

Fig. 1b Mesh of a resistor with knowledge of singularity

The discrete Poisson equation obtained by applying conventional finite differences has a local truncation error linearly proportional to the mesh spacing and the third partial derivatives of the electrostatic potential on a non-uniform mesh. By applying Scharfetter-Gummel finite differences we get for the discrete continuity equations a local truncation error linearly proportional to the mesh spacing and the sum of the first and second partial derivatives of the current density components (for the considered equation).

For the numerical treatment the righthand side of (4) is expanded in a

Taylor series around the point $(x + h_i, y + k_j)$:

$$\begin{aligned}\rho(x+h_i, y+k_j) &= \rho(x,y) + \\ &+ h_i\rho_x(x,y) + k_j\rho_y(x,y) + \\ &+ \frac{h_i^2}{2}\rho_{xx}(x,y) + \frac{h_i k_j}{2}\rho_{xy}(x,y) + \frac{k_j h_i}{2}\rho_{yx}(x,y) + \frac{k_j^2}{2}\rho_{yy}(x,y) + \\ &+ O(g_{i,j}^3)\rho'''\end{aligned} \tag{5}$$

where $g_{i,j} = \max(h_i, k_j)$, $\rho_x = \frac{\partial\rho}{\partial x}$ and $\rho_y = \frac{\partial\rho}{\partial y}$ and ρ''' derivatives of ρ of order 3 and higher.

In the discretized fomulation of (1)–(3) only the first term $\rho(x,y)$ is considered. The truncation error of (5) after the first term will be integrated over a rectangular domain around each point thus providing the following simple formula for a first order approximation of the local discretization error.

$$\begin{aligned}\Delta_\psi = &\int_{-k_{j-1}/2}^{k_j/2}\int_{-h_{i-1}/2}^{h_i/2} (\rho(x+\varsigma, y+\eta) - \rho(x,y))\; d\varsigma d\eta = \\ &A \cdot \Big(\frac{1}{4}(h_i - h_{i-1})\rho_x + \frac{1}{4}(k_j - k_{j-1})\rho_y + \\ &\frac{1}{24}(h_i^2 - h_i h_{i-1} + h_{i-1}^2)\rho_{xx} + \frac{1}{32}(h_i - h_{i-1})(k_j - k_{j-1})\rho_{xy} + \\ &\frac{1}{32}(k_j - k_{j-1})(h_i - h_{i-1})\rho_{yx} + \frac{1}{24}(k_j^2 - k_j k_{j-1} + k_{j-1}^2)\rho_{yy}\Big)\end{aligned}$$

$A = \frac{h_i + h_{i-1}}{2} \cdot \frac{k_i + k_{i-1}}{2}$ denotes the integration area, ρ_x stands for the partial derivative of ρ with respect to the x-direction.

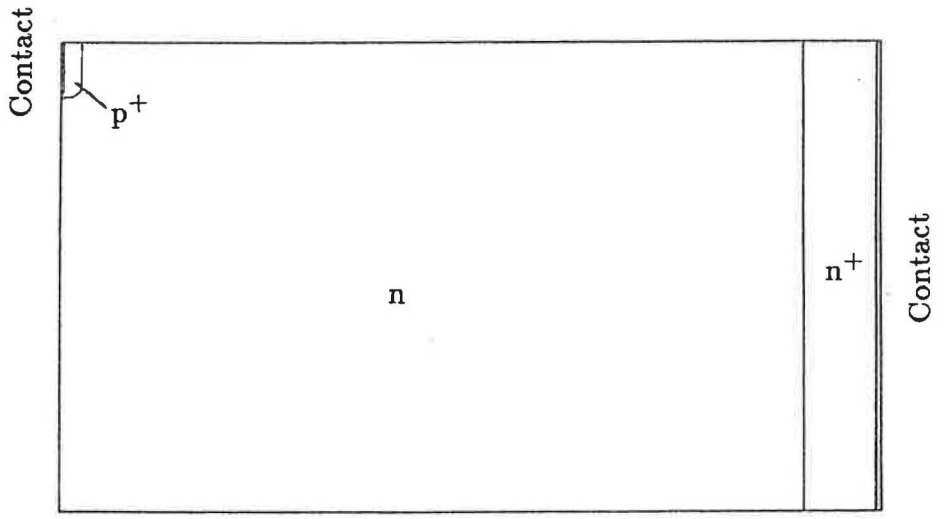

Fig. 2 Geometry and doping of a diode

In Fig. 2 the geometry and the doping of a diode is given. In Fig. 3 the *distribution* of the local discretization error of this diode can be seen (0.3V in backward direction). The values have been scaled to unity therefore it gives *no* information about the *quantity* of the error. As it could be expected the error is concentrated at the location of the singularity in the electric field while the error over the remaining device area is neglegible. An extension of our program in order to isolate these singularities by a special treatment in grid processing is under investigation.

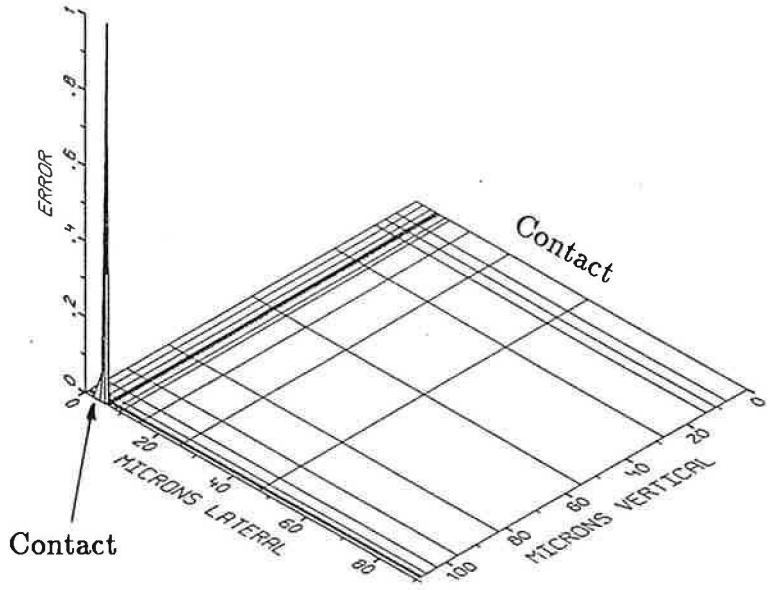

Fig. 3 Distribution of local discretization error of diode

Various numerical experiments have shown that the equidistribution of the local discretization error does not provide the optimal grid. Therefore some additional considerations have to be taken into account in order both to improve the ratio between the number of mesh points and the accuracy of the solution and to reduce numerical difficulties.

In the simulation of high voltage devices an additional criterion is applicable: The coupling of the discretized equations (1)–(3) is mainly determined by the Bernoulli function $B(x) = \frac{x}{e^x - 1}$ which is introduced by the discretization based on the Scharfetter-Gummel approach. x denotes the difference of the electrostatic potential at two neighbouring grid points divided by the thermal voltage U_T. A local decoupling of the equations because of vanishing values of B may lead to numerical difficulties. At low temperatures this effect becomes even worse.

Limiting B is in fact a restriction to ψ under equithermal conditions. It is well known that a rigorous restriction to the electrostatic potential is too strong because the local truncation error of Poisson's equation is linear proportional to the mesh spacing and the *third* partial derivatives of ψ. This means that in the case of no changes in the space charge the differences of the potential values do not affect the computational error. On the other hand the magnitude of B is of fundamental impor-

tance for elliptic and mixed problems where the solution is determined by the boundary conditions. This means that especially at Dirichlet boundaries (i.e. contacts) and in regions with varying space charge a local decoupling because of vanishing values of B has to be avoided by inserting new lines.

Another more physical criterion has to be taken into account. Particularly in high voltage breakdown simulations the net generation/recombination R gives good information for placing new points in the grid. It has turned out that in areas with $|R| > 10^{22}$ cm^{-3} s^{-1} new points have to be inserted because otherwise not all physical effects in the device can be observed. As minimum grid distance the mean free path of electrons in silicon (about $60 \cdot 10^{-8}$cm) should be taken. Furthermore by using this refinement criterion convergence speed of the Newton linearization scheme is significantly increased [5].

One more strategy should be mentioned which is of special importance for transient computations. For time dependent simulations the grid should change because the areas of interest move. In order to minimize the number of grid points for a desired accuracy it is necessary to remove points if they are not longer needed. But even in stationary computations this may give an advantage because a badly choosen initial mesh may be corrected.

Various tests have shown that removing *single points* from the grid will be very time consuming since the mesh has to be regularized again (assumptions about the ratio of the distances between two points a.s.o.). For this reason we investigate *lines* to be taken away. From theory we know about linear variation in the potential values and about the linear convergence rate. This means that removing a line will about double the discretization error in a first estimation. Therefore only lines with an error at each point which is less than half the allowed error (given by the desired accuracy) may be taken away.

In Fig. 4 a,b two grids for the stationary computation of the diode from Fig. 2 can be seen. For the grid shown in (a) (332 points) only the discretization error has been controlled without removing lines from the grid, for the grid shown in (c) (317 points) lines have been removed according to the mentioned criterion. In both cases the same stopping criterion and the same boundary conditions have been settled. It can clearly be seen, that the lines which have been inserted during the construction of the initial grid because of the gradient in the doping profile (particularly at the n-n$^+$-junction) could be removed since they are of no importance for this operating point (small voltage in backward direction).

The solution of (1)-(3) is either done by a modified version of Newton's algorithm (simultaneous solution of the equations) or by Gummel's algorithm (decoupled solution of the equations). In both cases it may occur that the iteration cycle does not converge.

From our knowledge it is not possible to give a generally applicable criterion for grid refinement in this case. A popular strategy is the analysis of the residual vector. In regions of the device with large resid-

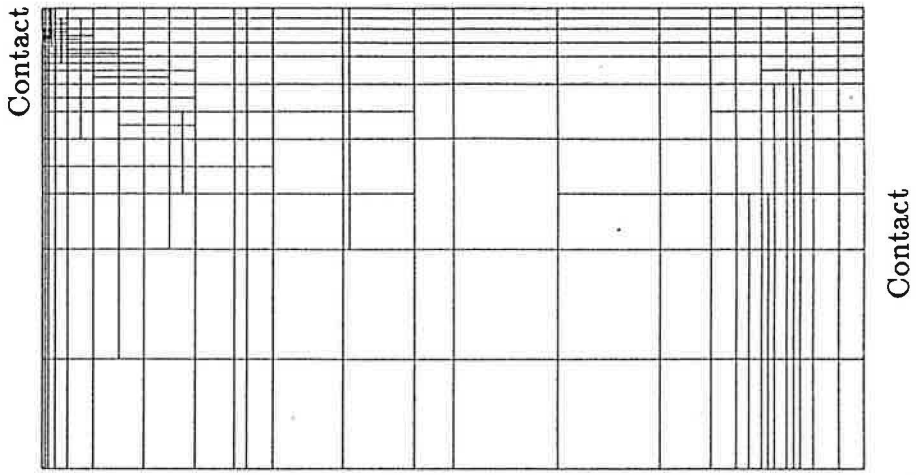

Fig. 4a Grid of diode without deletion of lines

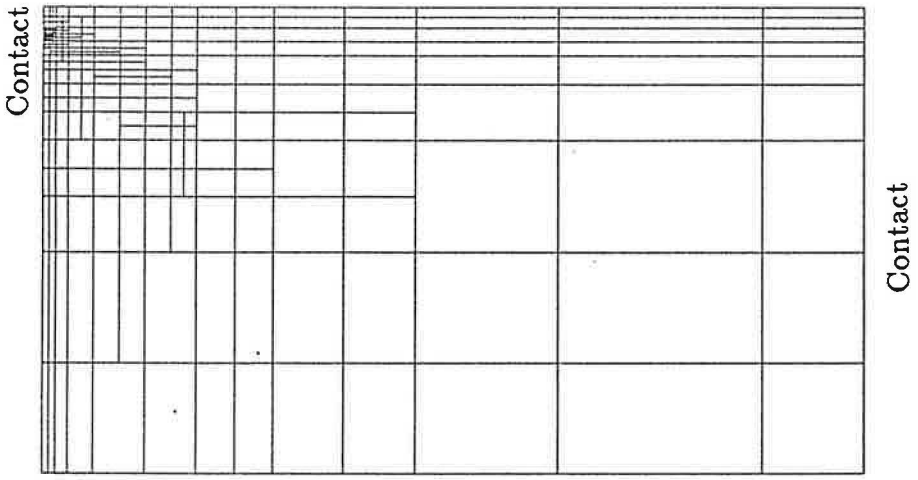

Fig. 4b Grid of diode with deletion of lines

uals new points are inserted. If the residual norm of the solution is near the desired accuracy this often enables convergence, but in other cases it sometimes fails. A more reliable method based on the solution of a set of Laplace equations is under investigation.

3. SELF–ADAPTIVE TIME GRID

In our simulator the implicit backward Euler method is utilized for the transient solution of the equations, because it is absolutely stable and no conditions for the time steps have to be taken into account. Since the orders of the time discretization and of the space discretization should be the same a method of linear order is sufficient.

In transient calculations all considerations about the space grid are

also applicable. But more than for the space grid it is very difficult to derive criteria for a self-adaptive time grid. This means that almost all considerations are based on heuristics or on physical properties.

Because the effects by the dielectric relaxation time are not analyzed in our program we take 1/100 of the maximum life time of carriers for the initial time step. This value has been established by numerical experiments.

The automatic time step control is almost equivalent to the estimation of the time and the space discretization error simultaneously. The space discretization error has been discussed in the last paragraph, the time discretization error is proportional to the change in the space charge. This can be written as

$$\Delta\rho = ||\rho_{t+1} - \rho_t|| = ||p_{t+1} - p_t - (n_{t+1} - n_t)|| \qquad (6)$$

Formula (6) can be computed very easily, furthermore it can directly be applied to the time grid. The time step is doubled if the change in the space charge is less than 10%, otherwise it is kept constant or reduced depending on the change in the applied voltages.

During transient calculations the local space discretization error is controlled only after each three time steps because otherwise this might lead to an exploding number of grid points. If an update of the space grid is performed, one has to watch the computational error which is introduced by the interpolation of the solution at the new points. In order to damp this error two quasi-zero time steps are introduced after each space grid update. It should be mentioned that the number of quasi-zero time steps depends on the order m of the time discretization scheme. From theory m intermediate time steps are sufficient, but it has turned out in numerical experiments that $m + 1$ steps give even better results [6].

4. CONCLUSION

We have presented strategies for both time and space grid control in device simulation illustrated by examples which have been computed with our device simulator BAMBI. Furthermore we have shown that the conventionally used criteria like limitation of the changes of the independent variables or equidistribution of the local discretization error are not sufficent to optimize the grid. An automatic time step width algorithm has been presented.

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