Locally adaptive multigrid method for 3D numerical investigation of semiconductor devices

P. Conradi, D. Schroeder
Dept. Techn. Electronics, TU Hamburg-Harburg
P.O. Box 90 14 03, D-2100 Hamburg 90, Fed. Rep. Germany

Abstract
The paper presents recent developments in the multigrid semiconductor device simulation program COGITO. A locally adaptive refinement strategy has been implemented. The electron and hole continuity equations have been incorporated into the solution procedure. Refinement criteria and interpolation topics are discussed in particular. The solution of a three-dimensional example problem is presented.

1 Introduction
In device simulation, the internal electronic behaviour of semiconductor devices is investigated by numerical analysis. The traditional semiconductor equations can be found in many textbooks, e.g. [1]. Due to the higher integration scale of VLSI devices, the demand to take three-dimensional factors into account will increase considerably in the near future. 3D simulations principally give rise to three problem areas:

- the development of numeric methods suitable for 3D computation,
- suitable device description (geometry in 3D, automatic grid generation); in this context an extension to the data transfer format EDIF [2] could prove to be helpful,
- suitable hardware for the support of the expensive computations.

In this paper, we will concentrate on the numeric problem. In 3D simulations considerable execution time bottlenecks ensue, since the total number of gridpoints increases to the 3rd power of the number of gridlines in one direction. Thus it will be necessary to search for numeric algorithms at an optimum level of complexity. It is a significant characteristic of the full multigrid method (FMG) to have a solution effort of O(n) at n discrete gridpoints. This may be true for the solution of Poisson's equation as well as for the class of diffusion problems [3]. The wide range of variation of the local parameters of the continuity equations in semiconductor physics, however, unfortunately increases the problem to find a solution with multigrid techniques.

Few authors are doing research on multigrid methods in device simulation, e.g. [3,4,5,6,7]. As a special feature the method implemented in our COGITO program [8] is based on representing discretizations as nested boxes like in [7], but uses a tree structured data organization for a discrete representation of 3D problems.

Fig. 1 shows the principle of the relation between space discretization and the hierarchical tree structure. Each transition from one tree node to its subnodes includes a division of the discrete boxes in a certain direction. Local refinement is possible by subdivision of selected boxes into subtrees. This binary tree data structure has been discussed in more detail in earlier papers [8,9].

In the following sections we present the latest developments particularly in the field of adaptive local refinement and the inclusion of the continuity equations.

2 Locally adaptive refinement strategy
To attain a higher grid resolution of important parts of the device in 3D without much more computational effort, we included a locally adaptive refinement strategy into the multigrid method. For that purpose, we constructed a recursive multigrid algorithm which operates on the tree data structure.

The algorithm automatically proceeds from a coarse grid into the (maybe only partially existent) finest grids. The heart of the algorithm is a recursive procedure which operates on a set of connected boxes, i.e. all boxes of equal size on a certain level in the tree structure (cf. fig. 1) that touch each other. This procedure allows to select the order of processing within the set (e.g. lexicographic order).
According to the multigrid method, the procedure first prolongates a correction to the solution from the next coarser grid. With this correction, a new approximation of the solution is computed and then relaxed. Subsequently, each of the connected boxes are checked if subboxes exist. In this case, the multigrid procedure is applied recursively to the set of boxes connected to the subbox, but only if these have not yet been processed. If no subboxes of a certain box are present, the refinement criterion (see below) is evaluated and subboxes are created according to the result. Finally, the defect and the solution are restricted from the finer level (if present), the solution is relaxed, and the defect is computed for the use on the coarser levels.

In order to check the necessity to refine a certain box, the following procedure has been used for our first attempts. The idea is: If the value of a certain quantity \( u \) in the box (e.g. the potential) is not well approximated by interpolation of the values in the neighbour boxes, the grid is too coarse and has to be refined. Thus the refinement criterion reads

\[
|u - u'| > \epsilon
\]

then refine box

where \( u' \) is the interpolated approximation and \( u \) is the value in the box itself. The preselected value of the parameter \( \epsilon \) controls the sensitivity of the criterion. As the interpolations are done separately in each of the coordinate directions, the criterion works direction oriented. With this approach we obtained acceptable results.

As pointed out in the literature [10,11], special care has to be taken in regions, where the meshsize of the grid changes abruptly. If the neighbour point on a grid line misses due to the termination of the line, it is not possible to use the regular difference star. A similar situation occurs in our hierarchical box discretisation at the boundaries of a locally refined region. Here, a box on a fine grid level adjoins to a box on a coarser level. The neighbour point does not lie in the direction of the coordinate axes, thus distorting the regular difference star.

To cope with these problems, we adopted a suggestion of P.W. Hemker [12]. At a boundary between different discretisation levels, the normal flux density (the displacement in the Poisson case, and electron resp. hole current in the case of the continuity equations) through the surface between the adjacent boxes is approximated on the level of the coarse grid, where the discretization is regular. Then it is assumed that the flux density on this surface is constant and valid on the finer grid level, too. This flux density is used for the discretization in the box on the fine level. A more advanced discretisation scheme - which better accounts for the tangential flux components on surfaces in irregular 3D grids - will be published later [13].

3 Treatment of continuity equations

For the treatment of continuity equations the variables electron and hole concentration are transformed into the Slotboom variables \( \xi_e \) and \( \xi_h \) [11]. We obtain

\[
\nabla \cdot (\xi_e \nabla \phi) + D \xi_e \nabla \phi - \xi_e \phi + N_D - N_A = 0, \quad (1)
\]

\[
\nabla \cdot (\mu_e \xi_e \nabla \phi) - R = 0, \quad (2)
\]

\[
\nabla \cdot (\mu_h \xi_h \nabla \phi) - R = 0. \quad (3)
\]

Note that the equations (2) and (3) are of the diffusion equation type.

The relaxation happens lexicographically and locally iterative in our implementation. A locally simultaneous solution procedure is under development.

In our multigrid approach, various informations have to be transferred between the different grids like

- prolongation (transfer coarse to fine) of the correction
- restriction (transfer fine to coarse) of residual and solution.

To obtain optimal results, the kind of interpolation has to be chosen in consistence with the governing equation. We temporarily installed linear interpolation of the Slotboom variables \( \xi_e \), \( \xi_h \).

Further variants as

- an interpolation approach after [7],
- the expression of interpolation through flux densities [13],
- usage of the solver itself for interpolation

are actually under development or test.

For brevity, example results are not given in this paper, but will be presented in the lecture.

4 A three-dimensional example with local refinement

As an example of a 3D simulation with adaptive refinement, we take a planar diode in thermodynamic equilibrium. In this case, eqs. (1 - 3) reduce to (1) with \( \xi_e = 1 \) and \( \xi_h = 1 \).

![Figure 2: Device Geometry](image)

Fig. 2 shows the geometry of our 3D-problem. The length of the device is 1 x 1 \( \mu m^2 \), the doping \( (N_D - N_A) \) is \( \pm 10^{17} \) cm\(^{-3} \), respectively. At the contacts we assume charge neutrality and at the semiconductor boundaries we place homogeneous Neumann boundary conditions. The coarsest initial grid has 4 x 4 x 4 boxes.

Fig. 3 depicts the computed 3D grid in perspective top view with the contact areas shaded. Fig. 4 shows the potential distribution in the plane indicated in fig. 3. The potential is displayed as a constant level in the finest boxes. Thus, the refinement of the discretisation becomes visible. Note the fine resolution of the steep potential gradients in the space charge region, the refinement in the main direction of the gradients, and the coarse grid in those regions where the potential is nearly constant.

In uncritical regions the number of boxes of the refined structure was effectively reduced compared to the regular structure that equally resolves the critical regions.

5 Conclusion

The conception of using multigrid techniques in semiconductor device simulation could be validated after the implementation in
COGITO by comparing the simulation of simple standard devices with well-known results. It can be stated that the Poisson equation in one up to three dimensions for the zero current case can be solved. Steep gradients are well resolved by adaptive refinement. The full classical equation system including the continuity equations could be solved in one dimension under a selected bias.

Under work are:

- mixed boundary conditions (e.g. for oxide),
- special interpolations for current equations,
- refinement strategy with regard to all three unknowns in common,
- continuity equations for 3D.

The authors are indebted to M. Weber for the provision of the local relaxation procedures.

References