Investigation of Vector Discretization Schemes for Box Volume Methods

O. Triebl and T. Grasser

Christian Doppler Laboratory for TCAD in Microelectronics at the Institute for Microelectronics
TU Vienna, Gusshausstrasse 27–29/E360, 1040 Wien, Austria
Triebl@iue.tuwien.ac.at

ABSTRACT

The application of the box integration method in Technology CAD environments is investigated. A particular difficulty arises from physical models like the impact ionization rate or the high-field mobility within the drift-diffusion carrier transport equations which rely on vector quantities. We discuss different methods how generation rates can be approximated in the box scheme and how the requirements for the applied vector discretizations are. Simulation results of devices operated near break-down are presented using implementations of the presented schemes. Advantages and disadvantages in respect to implementation, to errors, and to convergence behavior are presented.

Keywords: vector discretization, box method, tcad, snap-back

1 INTRODUCTION

Simulation environments for semiconductor devices, usually known as Technology CAD (TCAD) tools, model the device physics using basic semiconductor equations, consisting of partial differential equation (PDE) systems. Because of the complexity of the PDEs in non trivial semiconductor devices, analytical solutions are usually not available and numerical methods have to be applied. Consequently, discretization in time and space is necessary, where the latter is discussed in this paper.

The spatial discretization is represented by a mesh laid over the simulation domain, consisting of nodes, edges, and elements. In two dimensions (2D), the elements might be rectangular in orthogonal grids, or triangular in different types of structured and unstructured meshes. The extension to three dimensions (3D) leads to cuboids and tetrahedrons, respectively.

The discretization step transforms the non-linear PDE system that describes the carrier transport in semiconductor devices into a non-linear difference equation system. A solution of this equation system can be found for instance by using Newton's method.

In this work the drift-diffusion transport equations are used. The continuity equation reads

$$\nabla \cdot \mathbf{J}_\nu + s_\nu \mathrm{q} \frac{\partial \nu}{\partial t} = -s_\nu R, \tag{1}$$

where $\nu \in \{n, p\}$ is the electron (n) and the hole (p) concentration, respectively, $\mathbf{J}_\nu$ is the current density for the carrier type ν, $s_n = -1$, $s_p = +1$, q is the elementary charge and R is the recombination rate. The current relation is solved together with Poisson's equation

$$\nabla \cdot (\hat{\epsilon}\mathbf{E}) = \rho = q(p - n + C), \tag{2}$$

where $\mathbf{E}$ is the electric field, $\hat{\epsilon}$ is the permeability tensor, ρ the charge and C the net concentration of fixed charged particles, including donors and acceptors. The drift diffusion relation for the current density reads

$$\mathbf{J}_\nu = \mathrm{q}\nu\mu_\nu\mathbf{E} - s_\nu \mathrm{q} D_\nu \nabla\nu, \tag{3}$$

where μ_ν is the mobility and D_ν the diffusivity for each carrier type. Using (3) and the relation $\mathbf{E} = -\nabla\psi$, where ψ is the electrostatic potential, the vector quantities $\mathbf{J}_\nu$ and $\mathbf{E}$ can be eliminated and the remaining unknowns are n, p and ψ. This avoids vector quantities as unknowns in the equation system under investigation. Vector quantities are usually calculated in a post-processing step after each Newton iteration. However, those non-scalar values are needed in many physical models, like high-field carrier mobility or impact ionization rate models, which might have influence on the simulations results as well as on the convergence behavior of the iterative solution process.

There is no unique definition for the computation of vector quantities in a discretized system. 1D discretizations along edges can be interpreted as projections of the unknown field vector. A linear discretization like it is used for the electric field gives in a triangular element a unique solution for the field vector. Other quantities like the current density require non-linear discretizations which cannot be assembled straight-forwardly so that there is no distinct solution available. Different proposals are discussed in this paper in the context of calculating the impact ionization carrier generation rate.

2 DISCRETIZATION

The main discretization scheme used in this work is the box integration method [1] which is summarized in the next subsections.

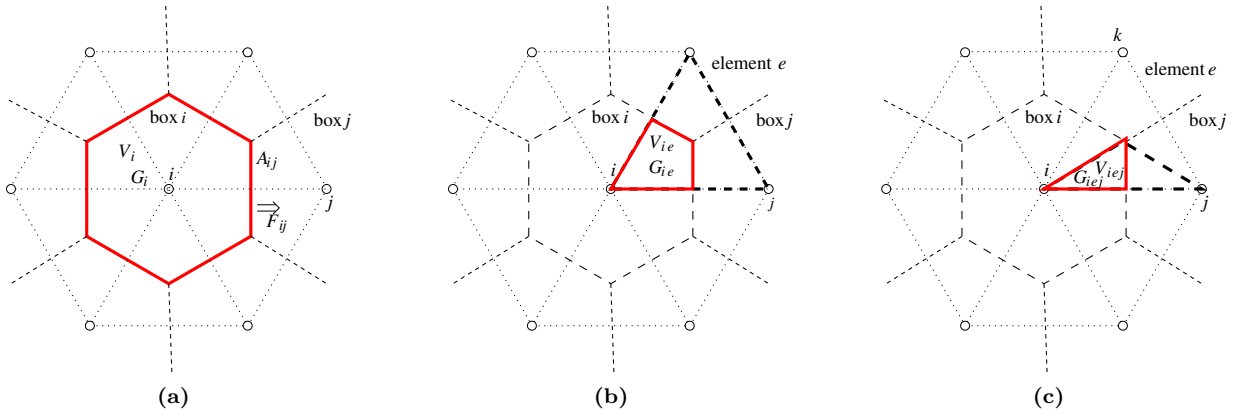

Figure 1: The Voronoi box i with its associated triangular elements. Area of constant generation term is shown for the box based methods (a), the element based methods (b), and the method proposed by Laux [4] (c).

2.1 Box Method

The basic discretization step concerns the divergence operation $\nabla \cdot \mathbf{F} = G$, with a flux density $\mathbf{F}$ and a generation term G $(= -R)$. Since (1) and (2) are of this form, integration over a volume V_i and application of the Gauss theorem gives

$$\oint_{\partial V_i} \mathbf{F} \cdot \mathrm{d}\mathbf{A} = \int_{V_i} G \mathrm{d}V, \tag{4}$$

where $\mathbf{A}$ is the outwardly oriented surface of the box volume.

Discretization of (4) allows one to write the left hand side as a sum of all fluxes leaving the box through the area ∂V_i which can be split into flat box boundary areas A_{ij}. A 2D representation of a box with its neighbors is depicted in Fig. 1a, where F_{ij} is the projection of the flux density onto the edge from box i to box j. This leads to the box integration method as it is used throughout this work:

$$\sum_{j \in \mathrm{N}_i} F_{ij} A_{ij} = \int_{V_i} G \mathrm{d}V, \tag{5}$$

where N_i is the set of all neighboring boxes. There are basically two sets of information necessary to describe the geometry for the box integration method: First, a list of all boxes together with the coordinates of the central nodes and the volume of the boxes, and second, a list of the connections between the boxes, the connecting edges, together with their edge lengths (d_{ij}) and surface areas (A_{ij}). This information is called the unstructured neighborhood information. It has to be noted that no more information about the elements is necessary, which leads to an independence of the element shape. Additionally, this type of information is independent of the problem dimension, which allows one to use the same program code for 1D, 2D, and 3D device geometries.

The surface area A_{ij} between two boxes i and j is delimited by the circumcircle centers and is needed to calculate the flux between two boxes. The center points have to be positioned inside the elements, otherwise the flux area would be negative. Therefore the mesh has to fulfill the Delaunay criterion.

2.2 Generation Integral

Physical models used in the drift-diffusion framework are often based on vector quantities. This is because the microscopic scattering rates which actually depend on the distribution function have to be approximated using the electric field, the current density, and the driving force. This is particularly true for the impact ionization generation rate, which can be calculated like in [2]: $G^{\mathrm{II}}(\mathbf{E}, \mathbf{J}) = \alpha_n |\mathbf{J}_n|/\mathrm{q} + \alpha_p |\mathbf{J}_p|/\mathrm{q}$, where $\alpha_\nu = \alpha_\nu^\infty \exp(-(E_\nu^{\mathrm{crit}}/|\mathbf{F}_\nu|)^{\beta_\nu})$. The calculation of the generation rate is therefore tightly bound to the discretization of vector quantities.

Different approaches have been published for the calculation of the generation integral on the right hand side of (5), three methods are discussed in this work. All of them assume the generation rate to be constant on a certain part of the box volume, which always requires an accompanying method for estimating vectors on the same volume. One approach to this problem is to assume the generation rate to be constant within one element. In this case, the generation integral for one box volume is assembled using contributions from each element attached to the box (see Fig. 1b):

$$\int_{V_i} G \mathrm{d}V \approx \sum_{e \in \mathrm{E}_i} G_{ie} V_{ie}, \tag{6}$$

where E_i is the set of all elements that contribute to the volume V_i. The rate calculated in one element is the same for all boxes the element is part of. This requires constant vector quantities in the whole element (see i.e.

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061844 Vol. 3, 2007

[3]). Some implementations associate different current densities for each edge pair and do not assume it to be constant within the whole element. In this case there are independent rates for each box the element is contained in, but (6) can still be used.

Another approach for the calculation of the impact ionization rate on triangular meshes has been proposed by Laux [4], where each element is split into three triangular regions, so called avalanche regions. The calculation delivers three different generation rates, each associated to one edge (see Fig. 1c). Therefore, the summation for the generation integral in the box volume requires one to consider two contributions from each element to one box:

$$\int_{V_i} G \mathrm{d}V \approx \sum_{e \in \mathrm{E}_i} \left(G_{iej} V_{iej} + G_{iek} V_{iek} \right). \tag{7}$$

The last approach discussed in this work assumes a constant generation rate in the whole box volume, which reduces the generation integral to a simple scalar product:

$$\int_{V_i} G \mathrm{d}V \approx G_i V_i. \tag{8}$$

Beside the simple assembly of the integral per box, this method has certain other advantages. The assumption of all scalar and vector quantities being constant within the box allows one to calculate only one rate for the whole box, which means that there is no additional geometry information for the assembly necessary. This results in a dimension and element shape independent implementation, which perfectly agrees with the box integration scheme in (5).

3 VECTOR DISCRETIZATION

As already stated above, there is no unique definition for the calculation of vector quantities in discretized systems. The main issue with vector quantities is that there are commonly only edge wise projected 1D discretizations available which have to be reassembled. The electric field for example is discretized with a finite difference approximation using the potentials on both ends of an edge and the current density is usually discretized using the non-linear Scharfetter-Gummel discretization [5].

In the previous section different volume parts that are used for the calculation of constant generation rates were discussed, each requiring a scheme for a constant vector approximation. We focus on the needs of the box based scheme (8) which requires a vector that is constant within the whole box volume. Two approaches that can be used for this task were summarized in [6]. The first one, scheme A, reads as

$$\mathbf{F}_i = \frac{1}{2V_i} \sum_{j \in \mathrm{N}_i} A_{ij} \mathbf{d}_{ij} F_{ij}, \tag{9}$$

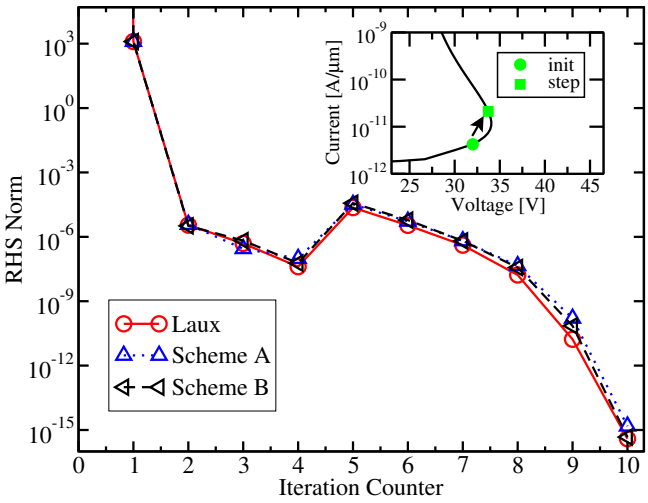

Figure 2: Convergence progress in a device with a 2D $\mathrm{n}^+\,\mathrm{p}\,\mathrm{n}\,\mathrm{n}^+$ structure operated near first break-down. The schemes show only marginal influence on the convergence behavior. The inset shows the initial and solution operating points for the two current level steps.

while the second one, scheme B, as

$$\mathbf{F}_i = \mathbb{M}_i^{-1} \sum_{j \in \mathrm{N}_i} \frac{A_{ij}}{d_{ij}^2} \mathbf{d}_{ij} F_{ij}, \tag{10}$$

using

$$\mathbb{M}_i = \sum_{j \in \mathrm{N}_i} \frac{A_{ij}}{d_{ij}} \mathbf{e}_{ij} \otimes \mathbf{e}_{ij}. \tag{11}$$

$\mathbf{d}_{ij}$ is the vector pointing form mesh point i to j, $d_{ij} = |\mathbf{d}_{ij}|$ and $\mathbf{e}_{ij} = \mathbf{d}_{ij}/d_{ij}$. $\mathbb{M}_i$ is called the geometry matrix and has to be calculated once for a non adaptive mesh. Both vector discretization schemes only require the unstructured neighborhood information, therefore the same geometrical information as for the box integration (5) is needed.

4 RESULTS

The two vector discretization schemes described in (9) and (10) and the scheme proposed by Laux [4] where implemented and used to calculate the impact ionization rate. The generation integral was assembled using (7) and (8), respectively. The implementation of the scheme by Laux is only limited to 2D domains using triangular meshes, whereas the two other schemes are dimension and mesh independent and the same program code can be used for 2D and 3D simulations.

Simulation results from two devices are presented: A diode which was selected to investigate effects in a simple device with only one relevant dimension and a parasitic $\mathrm{n}^+\,\mathrm{p}\,\mathrm{n}\,\mathrm{n}^+$ structure of a smart power device with a significant influence of the second dimension where cho-

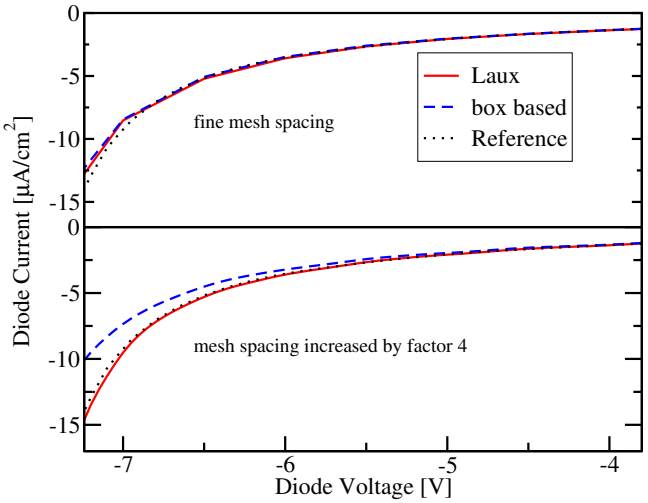

Figure 3: Comparison of the simulation results for a reverse biased diode near break-down using an equidistant mesh. A high mesh density leads to high accuracy for all schemes. Increasing the mesh spacing shows that the scheme by Laux gives better results because of the lower quantization error.

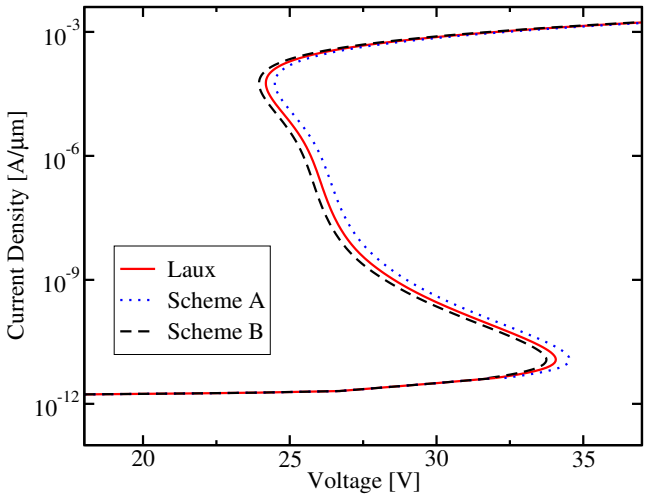

Figure 4: Comparison of simulation results of an $n^+ p n n^+$ structure operated near first break-down. The scheme from Laux gives the most accurate result compared to simulations using a higher mesh density (not shown).

sen. The diode is investigated in reverse biased operating condition, the parasitic bipolar smart power structure is simulated in snap-back, a state the device can be driven in during voltage peaks on the power line.

The influence of the vector discretization scheme on the convergence behavior was compared. Only very little differences were noted and no trend favoring one or another scheme was observed. The convergence process for a numerically critical current level step at the triggering phase of the snap-back in the smart power device is depicted in Fig. 2. It can be clearly seen, that the choice of discretization method has only very little influence, despite of the critical simulation step.

However, the mesh dependence of the results was observed to be higher for the box based discretizations. Using a high mesh density leads to comparable results for all three discretization methods, but using an increased mesh spacing, the results using Laux' scheme change very little, whereas the two box based schemes show large deviations. In Fig. 3 an example using the diode clearly shows that an increased mesh spacing leads to a shift of the break-down voltage using the box based schemes, whereas only a very small shift is observed using the scheme by Laux.

Also shown are results for the snap-back simulation in the smart power device which show deviations between the three schemes (Fig. 4). The two box based schemes again show a voltage shift in comparison to the scheme by Laux, which fits well to the solution from a high mesh density (not shown in the figure). The reason for the stronger mesh dependence can be found in the implicitly finer mesh used in Laux' scheme.

5 CONCLUSIONS

Discretization schemes for vector quantities together with the calculation of generation rates within the box integration method have been presented. Here, the assumption of a constant generation rate using constant vector quantities inside a box volume is of special interest. Implementations of two schemes using this assumption were compared to a scheme by Laux which uses an approach with smaller volumes of constant generation rate. Despite the lower accuracy obtained, two advantages are introduced by the proposed box oriented schemes. These are the independence on the problem dimension and on the mesh type used, as long as the mesh fulfills the Delaunay criterion. These independencies are possible because only the unstructured neighborhood information is required.

REFERENCES

[1] R. Bank, D. Rose, and W. Fichtner, IEEE Trans. Electron Devices, 30, 1031–1041, 1983.

[2] S. Selberherr, *Analysis and Simulation of Semiconductor Devices* (Springer, Wien–New York, 1984).

[3] J. Bürgler, R. Bank, W. Fichtner, and R. Smith, IEEE Trans. Computer-Aided Design, 8, 479–489, 1989.

[4] S. Laux and B. Grossman, IEEE Trans. Electron Devices, 32, 2076–2082, 1985.

[5] D. Scharfetter and H. Gummel, IEEE Trans. Electron Devices, 16, 64–77, 1969.

[6] O. Triebl and T. Grasser, in *Intl. Semiconductor Conference* (Sinaia, Romania), 337–340, 2006.