VECTOR DISCRETIZATION SCHEMES BASED ON UNSTRUCTURED NEIGHBORHOOD INFORMATION

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Abstract *— In TCAD environments, a proper vector discretization in two or three dimensions is an important issue. Physical models like the impact ionization rate depend on vector quantities. Two discretization methods for Delaunay meshes based only on the unstructured neighborhood information are presented. Overall good convergence is achieved by applying these methods in a TCAD environment for the calculation of the driving force vector as well as the current density vector. An example simulation of an nMOS transistor in snap-back operation is presented.*

1. INTRODUCTION

In TCAD simulation environments the basic semiconductor equation set, consisting of partial differential equations (PDE), has to be solved using numerical methods [1]. The spatial discretization is described with a mesh laid over the simulation domain. The often used drift-diffusion model consists of three independent variables, that are the electrostatic potential (Ψ) and the electron and hole concentrations (n and p). The box integration method is most commonly used to describe such problems and is also utilized in this work [2]. The method is based on a formulation that considers fluxes F_{ij} leaving a Voronoi box i to a neighboring box j along a connecting edge d_{ij} via the surface area A_{ij} (see Fig. 1), where the flux F_{ij} is evaluated only with quantities from the two neighboring points i and j. With the summation of all those fluxes and by using a generation term (G_i) inside the box volume V_i, scalar quantities in each box i can be approximated with a description similar to (1).

$$\sum_{all\ neighbors\ j} F_{ij} A_{ij} = G_i V_i \qquad (1)$$

For the calculation of this discretization, the only geometric information necessary is the unstructured neighborhood information. This includes a list of all mesh points with their associated volume, together with a connectivity list with one entry for each connection where the associated distance d_{ij} and the area A_{ij} are stored. Because of the flexibility of this formulation, it is independent of the problem dimension.

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In the drift-diffusion model two types of fluxes are used, the dielectric flux and the electron and hole current. The dielectric flux is approximated using finited differences and the current density with the Scharfetter-Gummel discretization [3].

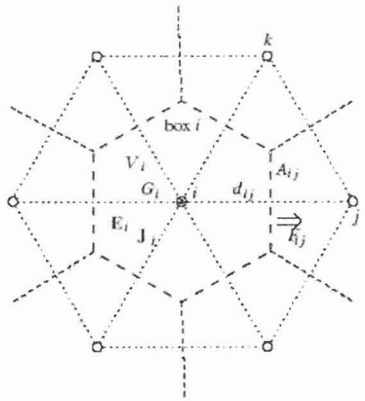

Fig. 1. Voronoi box i of mesh point i with connections to neighboring mesh points. The flux from box i to box j (F_{ij}) through the area A_{ij} is depicted. The vector quantities $\mathbf{E}_i$ and $\mathbf{J}_i$ are constant over the whole box i.

The system of the PDEs is commonly solved with an iterative Newton solver. The solution variables, i.e. Ψ, n and p, are quantities defined at the mesh points and are therefore known after each Newton iteration step. The fluxes from one box to a neighboring box are only defined at the box boundaries. Quantities like a field vector at a mesh point are normally determined in a post-processing step. Physical models like the carrier mobility $\mu(\mathbf{F})$ or the impact ionization rate G_n ($\mathbf{J}$,$\mathbf{F}$), depend on vector quantities $\mathbf{F}$ and $\mathbf{J}$ (driving force and current density for electrons and holes). Since the results form those models influence the solution variables, the vector discretization has a considerable impact on the simulations result and on the convergence behavior of the Newton solver. To achieve a good convergence behavior, it is necessary to add the derivatives of the vectors to the Jacobian matrix, especially when one of the named models dominates the device functionality.

Laux proposed a method for determine the impact ionization generation term on triangular meshes [4].

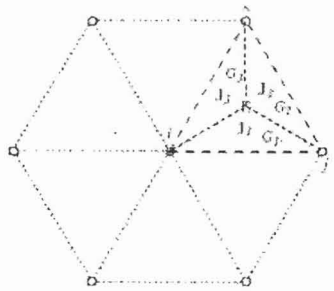

Fig. 2. Approach by S. Laux [4]: The electric field **E** is constant within one triangle and each triangle has one current density vector $\mathbf{J}_x$ for each edge.

The electric field is calculated inside a triangle by a linear interpolation of Ψ. In contrast, the current density inside a triangle is calculated individually for three different regions (see $\mathbf{J}_1$, $\mathbf{J}_2$, $\mathbf{J}_3$ in Fig. 2), by using a weighted linear combination of the Scharfetter-Gummel discretized currents along the edges: $\mathbf{J}_\nu = \mathbf{J}_\nu(J_{ij}, J_{jk}, J_{ki})$, $\nu \in \{1, 2, 3\}$. For the implementation of this scheme the triangles (in 2D) or the tetrahedrons (in 3D) have to be stored in addition to the unstructured neighborhood information. Furthermore, a different implementation for two- and threedimensional meshes is required.

In this work, two approaches are presented that assume all vector quantities constant over the whole box, consistent with the box integration method, and that only depend on the unstructured neighborhood information. They both aim to meet the following demands:

- simple coupling with box integration method;
- exact solution for homogenous fields;
- numerical stability.

After the derivation, a short discussion of the two approaches and a simulation of an nMOS transistor in snap-back will be presented, because in this operating condition the impact ionization dominates and the processed vector quantities will significantly influence the convergence of the Newton iteration.

2. DERIVATION OF VECTOR DISCRETIZATION SCHEMES

Two derivations for possible vector discretizations will be given in the following. The derivations are shown for the electric field, the generalization to gradient based fluxes is straight forward.

$$\mathbf{E} = -\nabla\Psi \Leftrightarrow \mathbf{J}_\nu = \pm q\nu\mu_\nu \nabla\varphi_\nu, \nu \in \{n, p\}. \quad (2)$$

A. SCHEME A

The first discretization scheme defines the projected component E^α in the direction e_α from the electric field **E** (3), where Ψ is the electrostatic potential.

$$E^\alpha = -e_\alpha \cdot \mathbf{E} = -\nabla\left((\Psi - \Psi_i)\, e_\alpha\right) \quad (3)$$

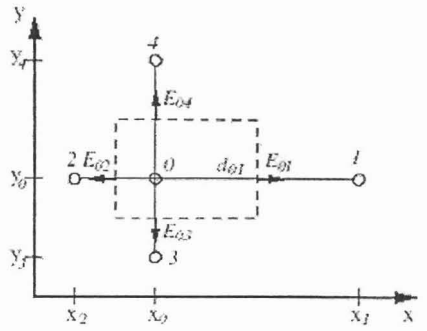

Fig. 3. Voronoi box of mesh point 0 with its neighboring points 1-4 in a non equidistant orthogonal mesh. The contributing field components E_{ij} from the edges are depicted.

By integrating over the box volume V_i and by approximating the integral with a sum, E_i^α in box i can be written as

$$E_i^\alpha = \frac{1}{V_i}\sum_j A_{ij}\frac{\Psi_i - \Psi_j}{2} e_\alpha \cdot e_{ij} \quad (4)$$

where the sum includes all neighbors j, A_{ij} is the surface between the two boxes i and j and Ψ_ν is the electrostatic potential in ν. By defining $\mathbf{E}_i = \left(E_i^x\ E_i^y\right)^T$, can be written as

$$\mathbf{E}_i = \frac{1}{2V_i}\sum_j A_{ij}\, d_{ij}\, E_{ij} \quad (5)$$

where d_{ij} is the distance between i and j ($d_{ij} = |\mathbf{d}_{ij}|$ with $\mathbf{d}_{ij} = (x_j - x_i\ y_j - y_i)^T$) and E_{ij} is the component of the electric field at the boundary between box i and j

$$E_{ij} = \frac{\Psi_i - \Psi_j}{d_{ij}} \quad (6)$$

B. SCHEME B

The second discretization scheme is an extension of the finite difference method and is based on a scheme proposed in [5]. Considering the box 0 in a non-equidistant orthogonal mesh depicted in Fig. 3 and its neighboring box 1 (not shown explicitly), the electric field along the edge d_{01} can be expressed as $E = -d\Psi/d_x$. At the boundary between the two boxes, i.e. the midpoint between 0 and 1, the finite difference method results in

$$E_{01} = \frac{\Psi_1 - \Psi_0}{d_{01}} \quad (7)$$

the same result as in (6). The electric field E_0^x in direction e_x at mesh point 0 is expressed with a linear interpolation (8), the same procedure is done for the component E_0^y (9).

$$E_0^x = \frac{\dfrac{E_{01}}{x_1 - x_0} + \dfrac{E_{02}}{x_2 - x_0}}{\dfrac{1}{x_1 - x_0} + \dfrac{1}{x_2 - x_0}} \tag{8}$$

$$E_0^y = \frac{\dfrac{E_{03}}{y_3 - y_0} + \dfrac{E_{04}}{y_4 - y_0}}{\dfrac{1}{y_3 - y_0} + \dfrac{1}{y_4 - y_0}} \tag{9}$$

An extension of this equation set, that also allows edges not aligned with the coordinate axis is

$$\frac{1}{x_j - x_i} \Rightarrow \frac{x_j - x_i}{(x_j - x_i)^2 + (y_j - y_i)^2} = \frac{x_j - x_i}{d_{ij}^2} \tag{10}$$

With the already specified vector $\mathbf{E}_i$ and with $e_{ij} = d_{ij}/d_{ij}$, a closed vector presentation can be formulated, where the area A_{ij} is used as a weighting factor.

$$\sum_j \frac{A_{ij}}{d_{ij}} (e_{ij} \otimes e_{ij})\, \mathbf{E}_i = \sum_j \frac{A_{ij}}{d_{ij}} e_{ij}\, E_{ij} \tag{11}$$

Note that (8) and (9) are still retained and can be extracted by using $e_{ij} = (1\ 0)^T$ and $e_{ij} = (0\ 1)^T$ respectively. $\mathbf{E}_i$ at the left side of (11) can be taken out of the sum and the remaining part of the sum results in a geometry dependent matrix, which is calculated once in the beginning of the simulation. This allows the convenient formulation of the final discretization rule for a vector $\mathbf{V}_i$ in point i shown in (12), using the geometry matrix M_i (13) and the geometry factor (14).

$$\mathbf{V}_i = M_i^{-1} \sum_j g_{ij}\, \mathbf{e}_{ij}\, V_{ij} \tag{12}$$

$$\mathrm{M_i} = \sum_j g_{ij}\, \mathbf{e}_{ij} \otimes \mathbf{e}_{ij} \tag{13}$$

$$g_{ij} = \frac{A_{ij}}{d_{ij}} \tag{14}$$

3. PROPERTIES OF THE DISCRETIZATION SCHEMES

Both derivations are based on the unstructured neighborhood information only, so they can be easily coupled with the box integration method.

The second demand, the exact solution for a homogenous fields $\mathbf{E} = \mathbf{E}_H$, with the electrostatic potential $\Psi(x) = -\mathbf{E}_H \cdot x$, was verified on scheme A (15) limited on orthogonal grids $d_{ij}/d_{ij} \in \{(\pm 1\ 0)^T, (0\ \pm 1)^T\}$.

$$\mathbf{E}_i = \frac{1}{2V_i} \sum_j g_{ij} (d_{ij} \otimes d_{ij}) \mathrm{E}_H = \mathrm{E}_H \tag{15}$$

For scheme B a general proof was performed (16).

$$\mathbf{E}_i = M_i^{-1} \sum_j g_{ij} (\mathbf{e}_{ij} \otimes \mathbf{e}_{ij}) \mathrm{E}_H = \mathrm{E}_H \tag{16}$$

The results of the discretization schemes with a linear electric field $E(x) = -2\alpha x$ and an quadratic electrostatic potential $\Psi(x) = \alpha x^2$ was investigated in one dimension. Using only the x-axis and the naming convention from Fig. 3, the discretization scheme A results in (17) and scheme B results in the exact solution (18).

$$E_{scheme\,A}(x_0) = -\alpha (x_1 - x_2) \tag{17}$$

$$E_{scheme\,B}(x_0) = -2\alpha x_0 \tag{18}$$

The error of scheme A depends on the the ratio d_{01}/d_{02} and results in

$$E_{scheme\,A}(x_0) = \frac{E_{\mathrm{scheme\,A}}(x_0)}{E(x_0)} = \frac{1}{2}\left(\frac{d_{01}}{d_{02}} + 1\right) \tag{19}$$

With a mesh distance ratio in the range [1/1.16 ...1.16], the error reaches 30%.

The discretization results and the error calculation for scheme A are valid for the vector at the mesh point.

In future work it has to be determined, if the mesh point itself is a good choice for adequate vector modeling over the whole box, expecially when it is shifted away from the center. Additionally, investigations for higher dimensions are necessary to find more results and comparison criteria for the two discretization schemes.

Analyzing the geometry matrix M_i in scheme B shows, that it results from a sum of symmetric matrices $e_{ij} \otimes e_{ij}$ whose determinants equal 0 and whose main diagonals are positive. The sum of symmetric matrices with positive main diagonals and non-negative determinants results in a symmetric matrix with positive main diagonal and a non-negative determinant. If at least two of the participating matrices are linear independent, the determinant of the geometry matrix is positive. As long as the Delaunay criterion is fulfilled, there are always linear independent edges for one box and the inverse geometry matrix can be calculated.

The introduction already stated that the derivatives on mesh points are needed for the Jacobian matrix. This makes it necessary, that the derived discretization schemes are also differentiable on quantities ξ_k associated to a mesh point k. This is indeed possible and one obtains for Schema A.

$$\frac{\partial \mathbf{E}_i}{\partial \xi_k} = \frac{1}{2V_i} \sum_j A_{ij}\, d_{ij}\, \frac{\partial E_{ij}}{\partial \xi_k} \tag{20}$$

and for Schema B

$$\frac{\partial \mathbf{E}_i}{\partial \xi_k} = M_i^{-1} \sum \mathbf{g}_{ij}\, \frac{\partial E_{ij}}{\partial \xi_k} \tag{21}$$

In both discretization schemes, the existence of $\frac{\partial E_{ij}}{\partial \xi_k}$, which is available in any device simulation based on the box integration method, is sufficient to calculate $\frac{\partial \mathsf{E}_{ij}}{\partial \xi_k}$.

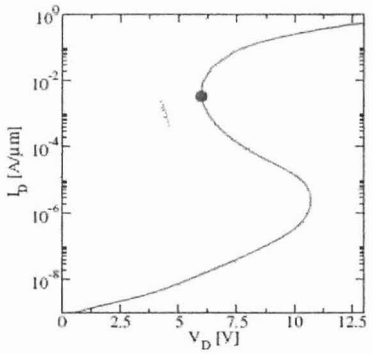

Fig. 4. Simulation result of an nMOS transistor in snap-back. A detailed 2D plot in the marked operating point is shown in Fig. 5.

4. EXAMPLE

To demonstrate the applicability of these discretization schemes, a two dimensional simulation with the discretization scheme B is presented. An nMOS transistor in snap-back is simulated where impact ionization is the dominating effect, and a physical model that strongly depends on vector quantities is used.
This generation term is one of the most challenging problems, especially when it dominates the device behavior. For modeling impact ionization in the driftdiffusion equation set, a modified version of the model [1] has been chosen

$$G^{II} = \alpha_n \left| \frac{\mathsf{J}_n}{q} \right| + \alpha_p \left| \frac{\mathsf{J}_p}{q} \right| . \qquad (22)$$

G^{II} is the impact ionization generation term on the right hand side of the continuity equation. $\mathbf{J}_n$ and $\mathbf{J}_p$ are the electron and hole current densities, q is the elementary charge and α_ν, $\nu \in \{n, p\}$, is defined as

$$\alpha_\nu = \alpha_\nu^\infty \exp\left(-\left(\frac{\mathsf{E}_\nu^{crit}}{\mathsf{F}_\nu} \right)^{\beta_\nu} \right), \qquad (23)$$

where α_ν^∞, E_ν^{crit} and β_ν are material dependent parameters. The difference to the model in [1] is, that the driving force $\mathbf{F}_\nu$ is used instead of the electric field. The simulations were performed with an adapted version of MINIMOS-NT [6], all derivatives of the impact ionization terms were calculated and added to the Jacobian matrix.

The device that was simulated is a standard nMOS transistor with gate length l_g = 1 µm and oxide thickness t_{ox} = 15 nm. During the simulation the source was grounded and the gate was fixed at a low voltage (V_G = 0.5V). The drain contact was first stepped with voltage control from 0V up to 10V, then the control was switched to a current control to simulate the snapback.

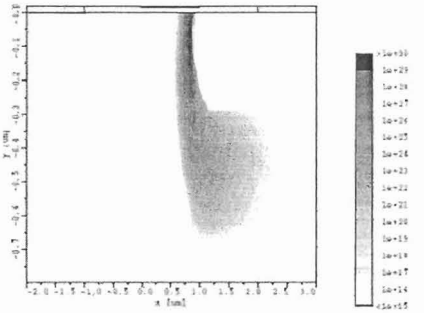

Fig. 5. 2D plot of the impact ionization generation rate at the operating point marked in Fig. 4.

The result of this quasi-stationary simulation can be seen in Fig. 4. The discretization scheme allowed to carry out the simulation in the snap-back region. A plot of a two dimensional cut through the device showing the impact ionization rate is depicted in Fig. 5. Note the big local differences near the drain region.

5. CONCLUSIONS

Two vector discretization schemes that seamlessly integrate in the box integration method were presented. Both schemes allow to be used on all mesh types, as long as the Delaunay criterion is fulfilled, so they can be used on orthogonal as well as on triangular meshes. The general formulation allows them to be used in 1D, 2D and 3D. An example simulation of an nMOS transistor in snap-back was presented, showing that this scheme can handle numerically challenging configurations very well.

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