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Box Method for the Convection-Diffusion Equation Based on Exponential Shape Functions

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Abstract

We present a derivation of exponential shape functions for the convection diffusion problem. The shape functions are defined for triangular elements and can be regarded as an extension of the one-dimensional Scharfetter-Gummel discretization scheme to two dimensions. The shape function varies exponentially in the direction of the element field vector and linearly in the direction orthogonal to the element drift velocity vector. A conservative discretization scheme is constructed by means of the box method. The resulting element matrix is not necessarily an M-matrix. A measure to stabilize the discretization is briefly outlined.

1 Introduction

With the advent of strain engineering in CMOS technology the modeling of carrier transport in anisotropic media has considerably gained in importance. Today's TCAD tools employ virtually exclusively the Scharfetter-Gummel (SG) discretization scheme for the convection-diffusion equation [1]. This scheme is derived assuming current conservation along the edges of a mesh. For certain applications, such as magneto-transport and transport in anisotropic media, however, the one-dimensional treatment of the edge currents is no longer sufficient and two-dimensional extensions of the SG scheme have to be sought. An established solution to this problem has been proposed in [2] and [3] and is known as the edge-pair method [4]. This method attempts to reconstruct a current density vector for a triangular element from three projections on the edges, whereby these projections are again determined by the one-dimensional SG expression. In this work an alternative method of extending the SG scheme to higher dimensions is pursued. Besides the coefficients of the discrete equation system the method also gives interpolation functions for the carrier concentration and the current density within the element

2 Extension of the Scharfetter-Gummel Scheme to two Dimensions

In analogy with the one-dimensional SG scheme which guarantees current conservation along an edge, one can demand current conservation within a simplex element in higher dimensions as well. Therefore, we look for analytical solutions of the carrier continuity

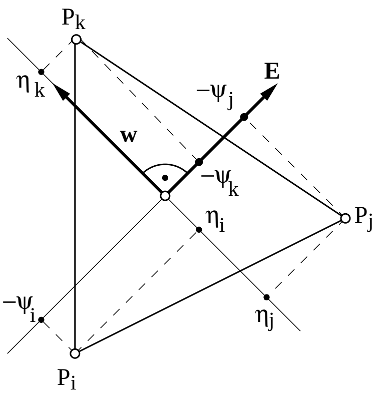

Figure 1: Local coordinate system spanned by **E** and **w**, which are orthogonal for an isotropic mobility. Also shown are the projections of the node vectors onto the coordinate axes.

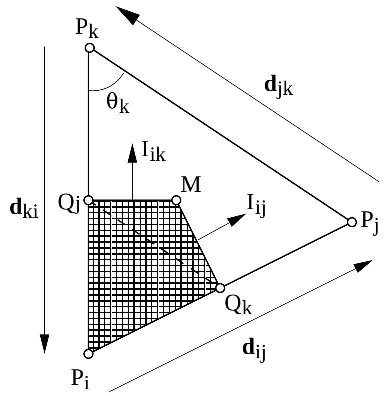

Figure 2: Intersection of the Voronoi box for node i and the element. The current sum $I_i = I_{ik} + I_{ij}$ can be obtained by integration of $\mathbf{J}(\mathbf{x})$ along the line $\overline{Q_j Q_k}$.

equation, $\nabla^T \hat{\mu}(n\mathbf{E} + U_T \nabla n) = 0$. For the purpose of discretization the mobility tensor $\hat{\mu}$ and the electric field vector $\mathbf{E}$ are assumed to be constant within the element. In two dimensions analytical solutions can be found by means of ansatz functions of the form $n_1(x,y) = A(x) + B(y)$ and $n_2(x,y) = C(x)D(y)$. Keeping only terms invariant under coordinate system rotation, one obtains a solution $n = n_1 + n_2$ containing three free parameters, which can be used as an interpolation function for triangular elements.

$$n(\mathbf{x}) = a + b\,\mathbf{w}^T\mathbf{x} + c\,\mathrm{e}^{-\mathbf{E}^T\mathbf{x}/U_T} \tag{1}$$

The vector $\mathbf{w}$ is orthogonal to the drift velocity, which implies $\mathbf{w}^T\mathbf{E} = 0$ for isotropic media and $\mathbf{w}^T\hat{\mu}\,\mathbf{E} = 0$ for anisotropic media. Vectors $\mathbf{E}$ and $\mathbf{w}$ define a non-normalized local coordinate system for a given triangle, as shown in Fig. 1. We define the local coordinates as $\psi = -\mathbf{E}^T\mathbf{x}$ and $\eta = \mathbf{w}^T\mathbf{x}$. Within a triangle the concentration (1) varies exponentially in the $\mathbf{E}$ direction and linearly (pure diffusion) in the $\mathbf{w}$ direction. The coefficients a, b, c in (1) are linear functions of the node variables n_i, n_j, n_k, obtained by solving the linear equation system $n(\mathbf{x}_l) = n_l,\ l = i, j, k$. An interpolation function of the form (1) has already been used by Baliga and Patankar in a decoupled scheme [5]. Analytical solutions of the two-dimensional continuity equation were also reported in [6]. In that work shape functions with four free parameters were sought, and rotationally variant terms were retained.

From (1) the current density vector is readily derived as $\mathbf{J}(\mathbf{x}) = q\hat{\mu}\left[(a + b\,\mathbf{w}^T\mathbf{x})\mathbf{E} + b\,\mathbf{w}\right]$. The current density is constant in the $\mathbf{E}$ direction and varies linearly in the $\mathbf{w}$ direction. To construct a box discretization scheme we consider the intersection of the Voronoi box for node i with the triangle i, j, k (Fig. 2). One needs to determine the normal currents I_{ik} and I_{jk} through the boundary patches $\overline{Q_j M}$ and $\overline{M Q_k}$, respectively. Because of current conservation the current sum $I_i = I_{ik} + I_{ij}$ is independent of the position of the circumcenter M and can directly be obtained by integrating the normal component of $\mathbf{J}(\mathbf{x})$ along the line $\overline{Q_j Q_k}$. The result is $I_i = (q\hat{\mu}/2)\left[(a + b\overline{\eta}_i)(\eta_k - \eta_j) + b(\psi_k - \psi_j)\right]$, where $\bar{\eta}_i = (2\eta_i + \eta_j + \eta_k)/4$ is the η coordinate of the midpoint between Q_j and Q_k. The coefficients a and b and hence I_i are linear functions of the node variables n_i, n_j, n_k. The current can be written as $I_i = q\hat{\mu}(c_{ii}n_i + c_{ij}n_j + c_{ik}n_k)$, where the off-diagonal coefficients are of the form

$$c_{ij}(\bar{\eta}_i) = \frac{1}{2\Delta}\left\{\left[u_k(\bar{\eta}_i - \eta_i) - u_i(\bar{\eta}_i - \eta_k)\right](\eta_k - \eta_j) + (u_k - u_i)(\psi_k - \psi_j)\right\} \tag{2}$$

$$c_{ik}(\bar{\eta}_i) = \frac{1}{2\Delta}\left\{\left[u_i(\bar{\eta}_i - \eta_j) - u_j(\bar{\eta}_i - \eta_i)\right](\eta_k - \eta_j) + (u_i - u_j)(\psi_k - \psi_j)\right\} \tag{3}$$

Here, $u = \mathrm{e}^{\psi/U_T}$ and $\Delta = u_i(\eta_k - \eta_j) + u_j(\eta_i - \eta_k) + u_k(\eta_j - \eta_i)$ is a determinant. Note that the transverse coordinates are linear functions of the node potentials, which can be written in matrix notation as $\eta = \mathbf{H}\psi$, where $\mathbf{H}$ is a constant element-dependent matrix, and $\eta = (\eta_i, \eta_j, \eta_k)^T$, $\psi = (\psi_i, \psi_j, \psi_k)^T$. Other off-diagonal coefficients related to the element under consideration are obtained from (2) and (3) by cyclic permutation of the indices, $i \to j$, $j \to k$, $k \to i$. Since the box method gives a conservative discretization scheme, the coefficient matrix exhibits vanishing column sums, $c_{ii} + c_{ji} + c_{ki} = 0$.

3 Discussion and Results

To discuss some properties of the coefficients (2) and (3) we choose a right angle triangle ($\theta_k = \pi/2$ in Fig. 2) and vary the field direction. The element field vector is represented as $\mathbf{E} = E(\cos\varphi, \sin\varphi)^T$. Fig. 3 shows that the coefficients associated with the hypotenuse oscillate around a mean of zero. While for the standard box method the coefficients c_{ij} and c_{ji} vanish exactly for $\theta_k = \pi/2$, with the exponentially fitted box method only the angular average of these coefficients vanish. A discretization scheme, however, requires the M-matrix property. Sufficient conditions are the vanishing column sum discussed above, and the non-negativity of the total coupling coefficients. Since the total coefficient c_{ij} is the sum of the coefficients of the two elements sharing the edge i, j, one of the two coefficients can be negative as long as the sum remains positive. If the sum is negative, one has to stabilize the discretization. For this purpose, a remarkable property of (2) and (3) can be utilized. We note that the coefficients are linear functions of the coordinate $\bar{\eta}_i$. If one now changes this coordinate within the limits of the triangle, the current density will change by $O(h)$, and the current I_i and the related coefficients by $O(h^2)$. Therefore, consistent with the $O(h)$ discretization one can deliberately change the $\bar{\eta}_i$ to some other coordinate η_i^*. It can be shown that the equation $c_{ij}(\eta_i^*) = 0$ has a solution $\eta_i^* \in [\eta_i, \eta_k]$, which lies inside the element. For the right angle triangle under consideration, the complementary coefficient (3) evaluated at η_i^* turns into the well-known Scharfetter-Gummel coefficient.

$$c_{ik}(\eta_i^*) = -\frac{\eta_k - \eta_j}{2(\psi_k - \psi_i)} B\left(\frac{\psi_k - \psi_i}{U_T}\right) = \frac{d_{jk}}{2d_{ki}} B\left(\frac{\psi_k - \psi_i}{U_T}\right) \tag{4}$$

This property shows the way how two coefficients associated with the edge pair of a certain node can simultaneously be made non-negative: The negative one is set to zero and the value of the complementary one is determined from (4).

The new discretization scheme has been implemented in MINIMOS-NT [7]. A fully-coupled Newton iteration is employed. The presented discretization and the one-dimensional SG method are compared for a pn-diode, shown in Fig. 4. The diagonal edges

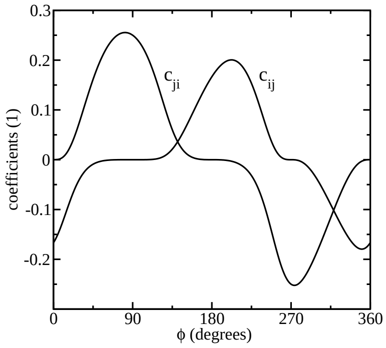

Figure 3: Coefficients as a function of the field direction for the hypotenuse of a right angle triangle with aspect ratio $d_{jk}/d_{ki} = 1$ and a maximum edge voltage of $Ed_{jk} = 2U_T$.

are either orthogonal (Mesh 1) or parallel (Mesh 2) to the average current direction. The current obtained from the SG discretization is independent of the orientation of the diagonal edges. Fig. 5 shows the differences of the currents from the exponentially fitted box method with respect to the SG current. The difference is pronounced for a coarse grid and vanishes for sufficiently fine grids. The applied voltage is $1V$.

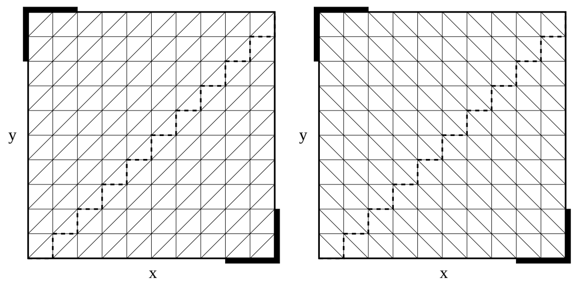

Figure 4: Pn-diode with square elements split into triangles. Left panel: Mesh1, right panel: Mesh2.

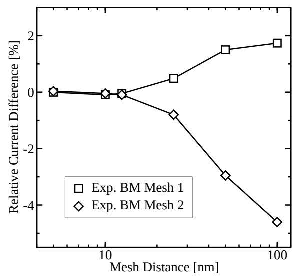

Figure 5: Relative difference with respect to the SG current.

Acknowledgments

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References

[1] D. Scharfetter and H. Gummel, IEEE Trans.Electron Devices **ED-16**, 64 (1969).
[2] W. Allegretto, A. Nathan, and H. Baltes, IEEE Trans.Computer-Aided Design **10**, 501 (1991).
[3] J. Egley and D. Chidambarrao, Solid-State Electron. **36**, 1653 (1993).
[4] H. Shao, Ph.D. thesis, Duke University, 1999.
[5] B. R. Baliga and S. V. Patankar, Numerical Heat Transfer **3**, 393 (1980).
[6] J. Machek and S. Selberherr, IEEE Trans.Electron Devices **ED-30**, 1083 (1983).
[7] *MINIMOS-NT 2.1 User's Guide*, Institut für Mikroelektronik, Technische Universität Wien, Austria, 2004.