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Construction of Stable Discretization Schemes for the Hydrodynamic Device Model

W. H. A. Schilders

Philips Research Laboratories
P.O.Box 80.000, NL-5600 JA Eindhoven, THE NETHERLANDS

Abstract

Several authors have reported numerical problems when simulating semiconductor devices using the hydrodynamic model. In this paper, the cause of these numerical problems is identified. Furthermore, a remedy consisting of adaptive quadrature rules is proposed. The resulting discrete schemes are stable, which is verified both theoretically and demonstrated through several examples.

1. Description of the model

The model considered in this paper has been described frequently in literature, and will therefore not be derived. It consists of the normal set of drift-diffusion equations, to which the following equations are added:

$$\nabla \cdot S_p = E \cdot J_p - Rw_p - p\frac{w_p - w_0}{\tau_w^p}, \tag{1}$$

$$\nabla \cdot S_n = E \cdot J_n - Rw_n - n\frac{w_n - w_0}{\tau_w^n}. \tag{2}$$

The energy flux densities are expressed in terms of the carrier temperatures, as follows:

$$S_p = -\kappa_p \nabla T_p + \frac{1}{q}(w_p + kT_p)J_p, \tag{3}$$

$$S_n = -\kappa_n \nabla T_n - \frac{1}{q}(w_n + kT_n)J_n. \tag{4}$$

In the above, w_p and w_n are the average energies of the carriers and the coefficients κ_p, κ_n are usually modelled using the Wiedemann-Franz law:

$$\kappa_p = C_{WF} k D_p p, \qquad \kappa_n = C_{WF} k D_n n.$$

In addition, the expressions for the current densities contain an extra term (due to temperature gradients) as compared to the classical drift-diffusion expressions:

$$J_p = -qD_p \nabla p + q\mu_p p E_p - qD_p^T p \nabla T_p, \tag{5}$$

$$J_n = qD_n \nabla n + q\mu_n n E_n + qD_n^T n \nabla T_n, \tag{6}$$

in which the thermal diffusion coefficients are often modelled by

$$D_p^T = \frac{D_p}{T_p} = \frac{k}{q}\mu_p, \qquad D_n^T = \frac{D_n}{T_n} = \frac{k}{q}\mu_n$$

2. The cause of numerical problems

The model described in the previous section is discretised using the finite volume method (or: box method). This means that, after a mesh (rectangular or triangular) has been constructed, each of the five partial differential equations is integrated over boxes around mesh points. In the resulting expressions, integrals of the form $\int \nabla \cdot Q$ (where Q is some vector quantity, for example J_n or S_n) are transformed into integrals over the boundary of the box. These boundary integrals can then be approximated by using low order quadrature rules, so that only normal components of the quantity Q at the midpoints between two nodes are required. These normal components are obtained by using Scharfetter-Gummel type expressions. This is very straightforward, and has been described in many publications.

The integrals of the right hand sides of the partial differential equations are usually approximated by applying the midpoint rule. Hence, the right hand sides only have to be evaluated at the mesh points. Both for Poisson's equation and the continuity equations, the midpoint rule can be shown to be the right choice in view of stability: the resulting discrete schemes yield non-oscillatory, physically relevant solutions, even for very coarse meshes. Because of the latter, adaptive meshing techniques starting from relatively coarse grids are possible. Clearly, this property would also be desirable for extended models, such as the hydrodynamic model. Unfortunately, this is not the case if the discretisation technique described is applied to equations (1)-(4). This is easily demonstrated using the following example, which was taken from [1]. For this problem (a pin-diode with a bias of 500 Volts), we display the discrete solution using 51 mesh points in Fig. 1. In addition to the oscillatory character of the discrete solution, we also found a rather slow convergence of the nonlinear solution process. These numerical problems were also observed for other devices; sometimes we even encountered severe cooling effects (carrier temperatures as low as 200 K).

Several authors have already expressed their opinion on the cause of these numerical problems. Some publications are devoted to a different discretisation of the normal components of S_p and S_n. This is, however, not the right angle of attack since it can be shown that the Scharfetter-Gummel type discretisation of these quantities leads to a system matrix with the right properties (M-matrix). Other authors have identified the discretisation of the term $E \cdot J_n$ as the cause of the problems, however, without giving a satisfactory explanation. Also, no adequate remedy has arisen from this observation.

After careful analysis of the system of equations, we found that the term $E \cdot J_n$ is indeed the cause of the numerical problems. More specifically, it is the additional term containing ∇T_n in the expression for J_n which causes instabilities. This can be verified mathematically by observing that, when expanding the term $E \cdot J_n$ into three terms, the use of the midpoint rule on the integrals over the boxes destroys the M-properties of the system matrix corresponding to the equations for the discrete carrier temperature T_n. A useful experiment to demonstrate this is the following: use a nonlinear solution strategy in which we first solve for the potential and the carrier concentrations (keeping the temperatures fixed), followed by the solution of the temperature equations. This iterative solution strategy may be viewed as a modified version of the wellknown Gummel's method. For the pin-diode used in Fig. 1, we find that the carrier temperatures are non-oscillatory after 1 iteration of this solution procedure. However, after 2 iterations we find 1 wiggle in the discrete solution and after 3 iterations there are 2 wiggles.

3. A stable discretisation scheme

The observation that the numerical problems are caused by the implicit dependence of the current density J_n on the carrier temperature T_n immediately points towards a possible remedy. Namely, the implicit dependence can be made explicit simply by expanding the term $E \cdot J_n$ into three terms and rewriting (2) in the form

$$\nabla \cdot S_n = qD_n E \cdot \nabla n + q\mu_n n \parallel E \parallel^2 + qD_n^T nE \cdot \nabla T_n - Rw_n - n\frac{w_n - w_0}{\tau_w^n} \qquad (7)$$

The third term in the right hand side of (7) being the only problematic term, we suggest to use the midpoint rule for all other terms, and a special quadrature rule for the integral of $qD_n^T nE.\nabla T_n$. We have developed an adaptive rule which takes into account the direction of the electric field E, full details of which will be given in a more extensive report (and at the conference). The effect of this rule on the coefficient matrices of the discretised system is such that contributions to the diagonal are non-negative, whereas contributions to the off-diagonal elements are non-positive. In this way, the M-matrix character [3] is conserved. In Fig. 2 we show the solution of the pin-diode obtained using this new quadrature rule, again with only 51 uniformly distributed mesh points.

4. Conclusion

In this paper, we have identified the true cause of the numerical problems encountered when using the hydrodynamic model. Having established, both theoretically and experimentally, that the implicit dependence of the current density on the gradient of the carrier temperature causes these problems, making this term explicit and using a different quadrature formula in the box integrals is shown to provide an adequate remedy. Although, in this paper, only a simple 1-d example has been given, experiments on 2-d examples have shown that the method performs well on more complicated devices (MOS-devices, bipolar transistors). The fact that the remedy has a sound mathematical basis is a guarantee that numerical problems are avoided irrespective of the grid size. In this respect, the proposed discretisation leads the way to adaptive meshing also for hydrodynamic simulations, without having to use extremely fine initial grids.

In addition to the non-oscillatory character of discrete solutions, we have found the nonlinear solution processes to converge much better. Indeed, vector extrapolation methods as used in [2] can be used to accellerate the modified Gummel method so as the obtain solutions even faster.

References

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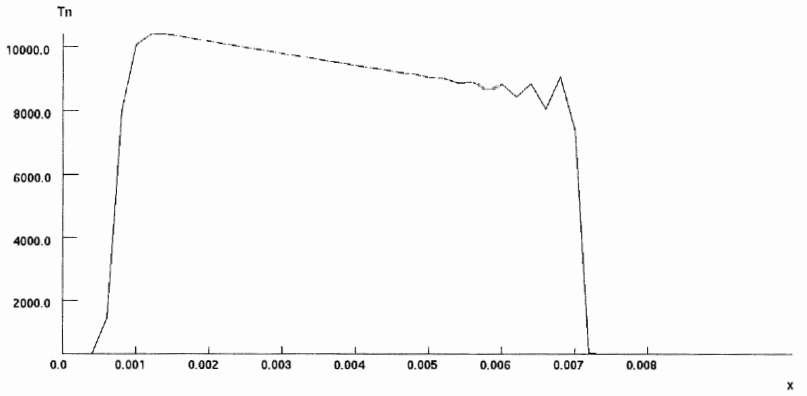

Figure 1: Electron temperature for pin-diode at -500 V using midpoint rule

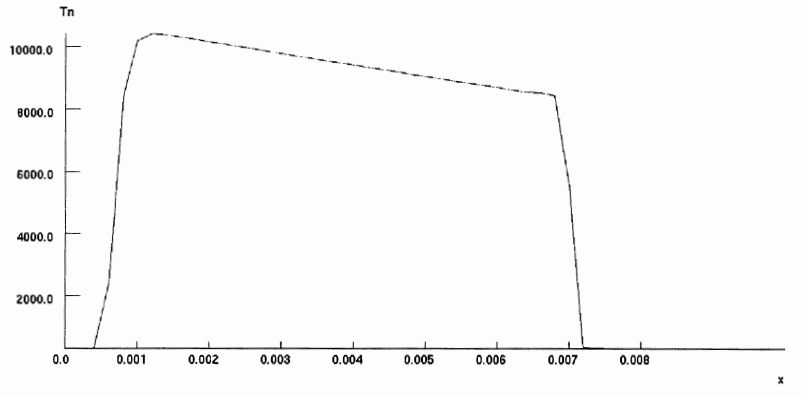

Figure 2: Electron temperature for pin-diode at -500 V using adaptive rule