ON THE INFLUENCE OF QUADRATURE RULES IN THE NEW SCHARFETTER-GUMMEL SCHEME

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1. Introduction

The numerical solution of the equations describing the steady-state behaviour of a semiconductor device is still a rather difficult problem. One of the difficulties is to find a suitable discrete formulation of the problem. Ordinary finite difference or finite element methods are not suitable and will give rise to non-physical oscillations in the hole and electron concentrations. In 1969, Scharfetter and Gummel designed a method which does not have this drawback (|2|). Since then, their method has been used by many device analysts to compute solutions for various semiconductor devices. Recently, a new version of the Scharfetter-Gummel scheme has been proposed (|1|). In this new method, quadrature rules play an important role. The aim of this paper is to analyse the influence of these quadrature rules in the new Scharfetter-Gummel scheme.

2. The box scheme

Consider the continuity equation for holes

$$\operatorname{div} J_p = -qR \tag{1}$$

where the hole current density is given by

$$J_p = \frac{q\mu_p}{\alpha} \text{ grad } p + q\mu_p \, p \text{ grad } \phi_p \tag{2}$$

Suppose we have a mesh of quadrilaterals which we would like to use to discretise equation (1). Then, for each mesh point M, we construct a box B around that point (see |1|).

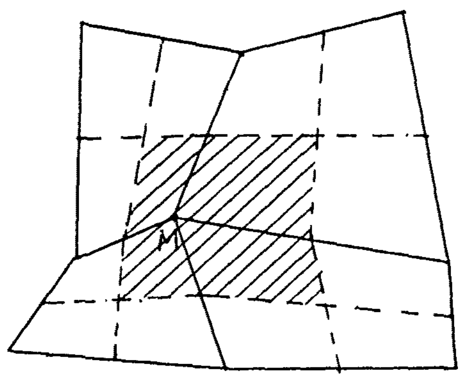


Figure 1

Then, instead of solving (1), we can try to solve

$$\iint_B \operatorname{div} J_p = \iint_B qR$$

Using Stokes' Theorem we can rewrite this as

$$\int_E J_p . \hat{n} = \iint_B qR \quad , \tag{3}$$

where E is the (octogonal) edge of box B and $\hat{n}$ is the unit outward normal. The discretisation of (3) is described in |1|: the right hand side is approximated by

$$q \text{ area}(B) \; R(M) \tag{4}$$

and the left hand side is approximated by

$$\sum_{i=1}^{8} I_i \tag{5}$$

where I_i is an approximation to

$$\int_{E_i} J_p . \hat{n} \tag{6}$$

Here, the E_i, $i=1,\ldots,8$ are the eight sides of the octogon B. Thus, we are faced with the problem to find a suitable approximation to the current flowing through an edge E_i. There are two difficulties here:

(i) find a suitable n-point quadrature rule with weights $w_1,\ldots,w_n$ and abcissae $\theta_1,\ldots,\theta_n$ and approximate (6) by

$$I_i = \sum_{k=1}^{n} w_k \, J^k_{p,\text{normal}} \tag{7}$$

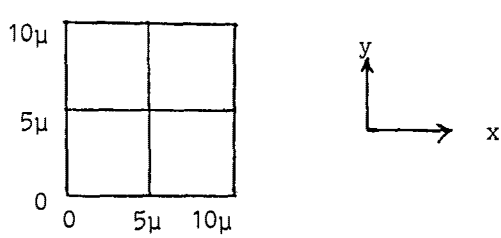
(ii) find an expression for $J^k_{p,\text{normal}}$ in (7) such that the resulting discretisation scheme is stable

Problem (ii) is discussed in |1| , where a new Scharfetter-Gummel scheme is proposed. Here, we will concentrate on problem (i).

3. Some simple examples

We illustrate the influence of quadrature rules on the solution of a problem with two examples. The first is a condensor, the second example is a diode. Both examples are one-dimensional, but we solve them as if they were two-dimensional. Thus, there should be no variation in the y-direction.

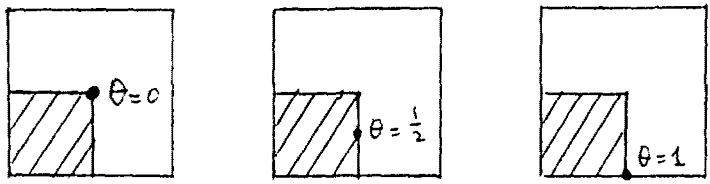
We solve both problems on a very coarse square mesh:



The quadrature rules we use are one-point rules of the form (compare (7) in section 2)

$$I_i = J_{p,normal}(\theta) \qquad ,$$

where θ is the normalized distance between the midpoint of a mesh and the nearest side of the mesh. Some examples:



Example 1: Condensor

We take the following problem:

$$\psi'' = 0 \quad \text{on} \quad |0, 10\mu|$$

$$\psi(0) = 0 \ , \ \psi(10\mu) = 1$$

We solve this problem on the square mesh given in figure 1. Below we show the solution of the discrete problem for the choices $\theta = 0$ and $\theta = 0.5$ .The graphs are marked with numbers 1, 2 and 3. '1' refers to the solution on the line $y = 0$, '2' to the solution on the line $y = 5\mu$, and '3' to the solution on the line $y = 10\mu$.

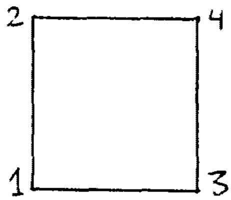
The boundary conditions can be given in several ways. We can choose to apply the boundary conditions in all points at the left and right side of the mesh, i.e. in the points marked 'X', or we can take a subset of these, marked 'O':

Case 1   Case 2

In figs. 2,3 the solution for case 1 is given, in figs. 4,5 the graphs for case 2 are displayed. Remark that the solutions in figure 4 are different from the solutions in the other three figures. This can be explained after some elementary calculations, the results of which are shown in Table 1. There we give the coefficients in the element stiffness matrix for the problem

$$\text{div grad } \psi = 0$$

on a square mesh



for several values of θ.

θ	1	2	3	4	
0	1/2	0	0	-1/2	
1/3	2/3	-1/6	-1/6	-1/3	(finite element)
1/2	3/4	-1/4	-1/4	-1/4	
2/3	5/6	-1/3	-1/3	-1/6	(high order fin.diff)
1	1	-1/2	-1/2	0	(finite diff.)

We see that, for certain choices of θ, we obtain the standard finite difference and finite element methods. Furthermore we see that we get a strange scheme ('chess board scheme') for $\theta = 0$, which explains the behaviour of the solution in figure 3.

Example 2: Diode

We take the following problem on $|0, 10\mu|$:

$$-\psi'' = q(p - n + D)$$

$$J_p' = -qR$$

$$J_n' = qR$$

$$J_p = -q\,\mu_p\, p\,\phi_p'$$

$$J_n = -q\,\mu_n\, n\,\phi_n' \quad ,$$

with boundary conditions

$$\phi_p(0) = \phi_n(0) = 0,$$

$$\phi_p(10\mu) = \phi_n(10\mu) = 0.1 \quad ,$$

and where ψ at the contacts is obtained from the requirement of charge neutrality. The doping function is taken to be

$$D(x) = \begin{cases} -10^{16} & \text{for } x < 5\mu \\ 0 & \text{for } x = 5\mu \\ 10^{16} & \text{for } x > 5\mu \end{cases}$$

Furthermore, we took

$$\varepsilon = 11.7$$

$$\mu_p = \mu_n = 1000$$

$$R = 0$$

$$n_i = 1.22\ 10^{10}$$

We solve this problem on the same mesh as we used for example 1 but we only take case 2. The results of our calculations are shown in figures 6-11. We see that the choice $\theta = 0.5$ is the better one in all cases. This can be explained in a way similar to that in example 1.

4. Conclusion

We have given a brief discussion of the influence of quadrature rules in the new Scharfetter-Gummel scheme as introduced in |1|. The two examples in section 3 show that one has to be careful in choosing the abcissae for the quadrature rules in order to obtain a reasonably accurate solution. In some cases a wrong choice for the quadrature rule can give non-unique solutions or solutions that do not satisfy the discrete maximum principle.

References:

|1| S.J. Polak, W.H.A. Schilders, 'A characteristics box scheme for the singularly perturbed continuity equation', these proceedings (1984)

|2| D.L. Scharfetter, H.K. Gummel, 'Large-signal analysis of a silicon Read diode oscillator', IEEE Trans. E. Dev., vol. ED-16, pp. 64-77 (1969)

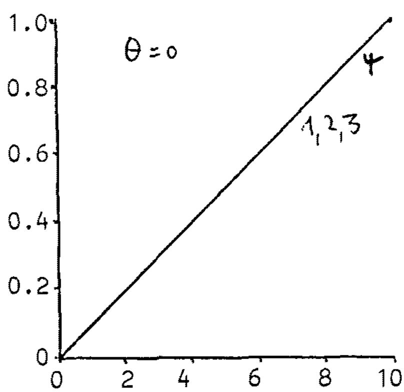


Figure 2

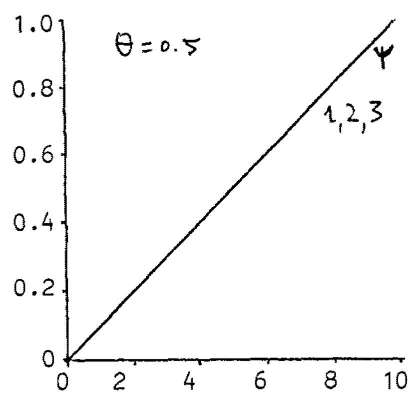


Figure 3

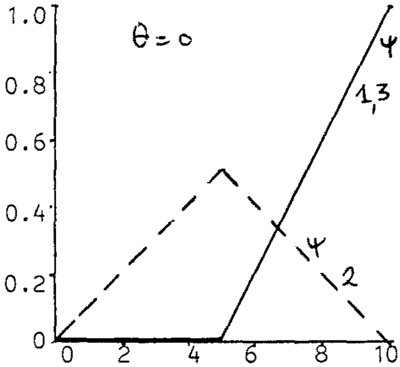


Figure 4

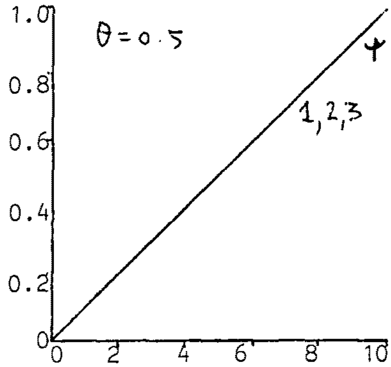


Figure 5

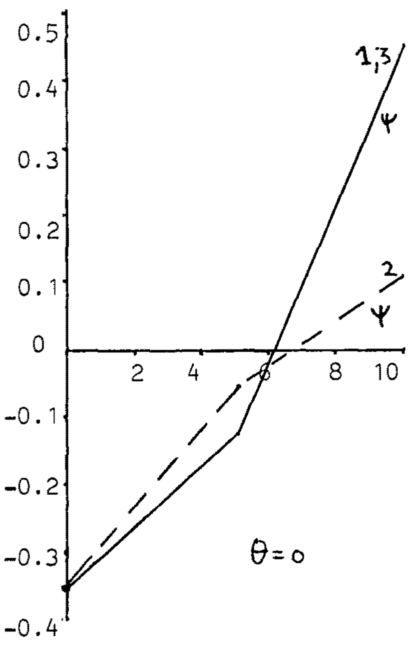


Figure 6

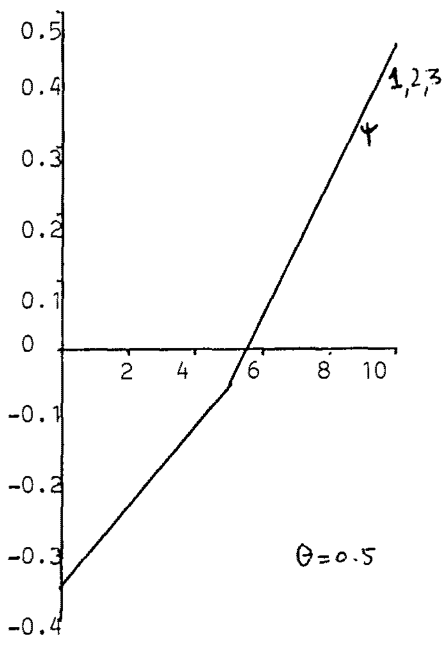


Figure 7

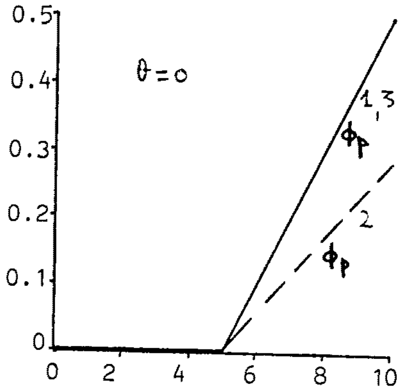


Figure 8

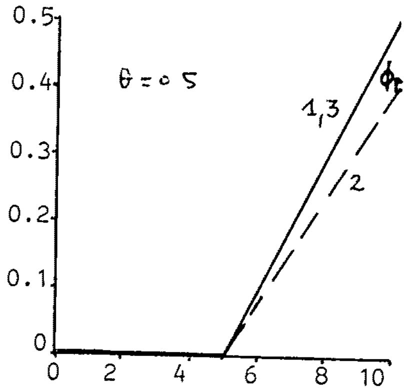


Figure 9

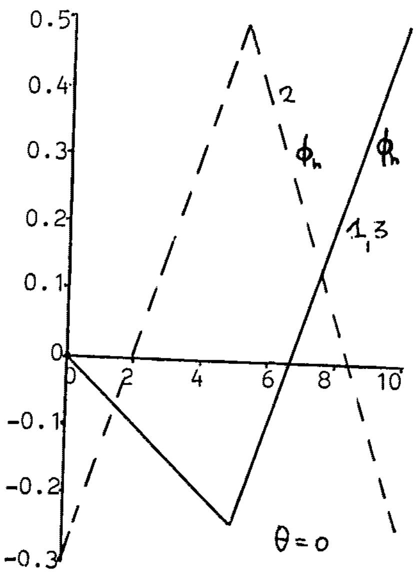


Figure 10

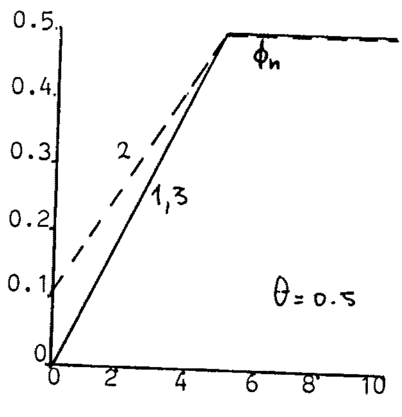


Figure 11