A MULTIGRID APPROACH FOR ONE-DIMENSIONAL SEMICONDUCTOR DEVICE SIMULATION

P.W.Hemker

CWI, Centre for Mathematics and Computer Science
P.O.Box 4079, 1009 AB Amsterdam, The Netherlands

1. Introduction

In this paper we give a brief description of a multigrid method for the solution of the 1-D semiconductor device modelling equations (drift-diffusion model). The essential part is the adaptation of the prolongation operator to the discretisation: an exponential interpolation is used to obtain a nested sequence of Scharfetter-Gummel discretisations.

Experiments with a model diode problem show that the usual multigrid efficiency can be obtained. A few iteration steps are sufficient to solve the discrete problems with truncation error accuracy.

A more comprehensive paper, with numerical results for the diode will be published elsewhere.

2. The equations

The equations modelling the steady semiconductor device are given by (cf. e.g. [3]),

$$-\nabla(\epsilon\nabla\psi) = q(p-n+D), \tag{2.1.a}$$

$$-\nabla(\mu_n(\nabla n - n\nabla(\alpha\psi+\log n_i))) = -R, \tag{2.1.b}$$

$$-\nabla(\mu_p(\nabla p + p\nabla(\alpha\psi-\log n_i))) = -R, \tag{2.1.c}$$

on $\Omega \subset \mathbb{R}^d$, $d=1,2,3$. The dependent variables ψ, n and p describe the electric potential and the electron and hole densities respectively; ϵ, the permittivity, and q, the elementary charge, are constant values, as is $\alpha = q/kT$, the inverse of the "thermal voltage". The doping D is a given (non-smooth) function of the independent space variable x. The electron and hole mobilities μ_n and μ_p as well as the net recombination- generation rate R generally are functions of x, ψ, n and p, and the intrinsic concentration n_i is a function of x. For simplicity, in this paper we consider only $R = 0$ and constant μ_n, μ_p and n_i. With these assumptions, (2.1) reduces to

$$-\nabla(\epsilon\nabla\psi) = qn_i(\bar{p}-\bar{n}+\bar{D}), \tag{2.2.a}$$

$$-\nabla(\mu_n(\nabla\bar{n} - \bar{n}\nabla(\alpha\psi))) = 0, \tag{2.2.b}$$

$$-\nabla(\mu_p(\nabla\bar{p} + \bar{p}\nabla(\alpha\psi))) = 0, \tag{2.2.c}$$

where $\bar{n} = n/n_i$, $\bar{p} = p/n_i$ and $\bar{D} = D/n_i$. Usual boundary conditions are either of Dirichlet type (at the contacts $\bar{p}\bar{n} = 1$, $\bar{p} - \bar{n} + \bar{D} = 0$, ψ prescribed) or of

Neumann type (cf.[3]).
Because of the large range of possible values for $\bar{n}$ and $\bar{p}$, it is convenient to introduce the quasi-Fermi levels as new variables:

$$\phi_n = \psi - \log(\bar{n})/\alpha = \psi - \log(n/n_i)/\alpha , \tag{2.3.a}$$

$$\phi_p = \log(\bar{p})/\alpha + \psi = \log(p/n_i)/\alpha + \psi . \tag{2.3.b}$$

In the new set of variables (ψ,ϕ_n,ϕ_p) the quantities all have the same dimension. Now (2.2) can be rewritten as

$$-\nabla(\lambda^2\nabla\psi) = e^{\alpha(\phi_p - \psi)} - e^{\alpha(\psi - \phi_n)} + \bar{D}, \tag{2.4.a}$$

$$-\nabla(\mu_n e^{\alpha\psi - \alpha\phi_n}\nabla(\alpha\phi_n)) = 0 , \tag{2.4.b}$$

$$-\nabla(\mu_p e^{\alpha\phi_p - \alpha\psi}\nabla(\alpha\phi_p)) = 0 , \tag{2.4.c}$$

where $\lambda^2 = \epsilon/qn_i$.
In view of (2.4), we introduce the notation $J_\psi = \lambda^2\nabla\psi$, $J_n = \mu_n e^{\alpha\psi - \alpha\phi_n}\nabla(\alpha\phi_n)$, $J_p = \mu_p e^{\alpha\phi_p - \alpha\psi}\nabla(\alpha\phi_p)$. Let $S \subset [L(\Omega)]^3$ be the set of all functions (ψ,ϕ_n,ϕ_p) such that $J_\psi, J_n, J_p \in H(\mathrm{div},\Omega)$, and $\bar{n},\bar{p} \in L^2(\Omega)$, then for arbitrary $(\psi,\phi_n,\phi_p) \in S$ and $\Omega_\alpha \subset \Omega$ we find

$$-\int_{\Gamma_\alpha} J_\psi \vec{\nu}\, d\Gamma = \iint_{\Omega_\alpha} (e^{\alpha(\phi_p - \psi)} - e^{\alpha(\psi - \phi_n)} + \bar{D})\, d\Omega , \tag{2.5.a}$$

$$-\int_{\Gamma_\alpha} J_n \vec{\nu}\, d\Gamma = 0 , \tag{2.5.b}$$

$$-\int_{\Gamma_\alpha} J_p \vec{\nu}\, d\Gamma = 0 , \tag{2.5.c}$$

where $\vec{\nu}$ the outward pointing normal at Γ_α, the boundary of Ω_α. This system of equations, together with the boundary conditions, is written in symbolic form as

$$N(q) = r(q), \tag{2.6}$$

where $N: S \to V = [L^2(\Omega)]^3$ is the nonlinear differential operator in the left hand side of eq.(2.4), $r(q)$ is the right hand side and q denotes the vector of unknown functions $q = (\psi,\phi_n,\phi_p)$.

3. The discretisation

To preserve the conservation character of the equations, for the discretisation of (2.4) we use a finite volume technique. We divide the interval $\Omega = (x_0,x_N)$ in disjoint *boxes* (i.e. intervals) $\Omega_i = (x_{i-1},x_i)$, $i = 1,...,N$. Inside each box Ω_i we select a point $x_{i-1/2}$ and for each box we approximate values of the variables ψ, ϕ_n and ϕ_p. To define a proper sequence of refining meshes as $N \to \infty$, we introduce a monotonously increasing $C^1[0,1]$-function $\gamma:[0,1] \to \Omega$ such that, for a fixed N, $x_i = \gamma(i/N)$. Another set of subintervals $\{D_i\}$ is introduced with $D_i = (x_{i-1/2},x_{i+1/2})$, $i = 1,...,N-1$, $x_{i-1/2} = (x_{i-1} + x_i)/2$ or $x_{i-1/2} = \gamma((i-1/2)/N)$, $D_0 = (x_0,x_{1/2})$, $D_N = (x_{N-1/2},x_N)$. These intervals form the set of *dual boxes*. Thus, for a given function γ, sets $\{\Omega_i\}_{i=1,...,N}$, and

$\{D_i\}_{i=0,...,N}$ are defined for an arbitrary $N \in \mathbb{N}$. The different discretisations are parametrised by $h = 1/N$. The set of boxes is denoted by $\Omega_h = \{\Omega_i | i = 1,2,...,N\}$.

A discrete representation $q_h \in S_h$ of the state of the semiconductor is given by the $3N$-dimensional vector $q_h = \{q_i\}_{i=1,...,N} = \{(\psi_i, \phi_{n,i}, \phi_{p,i})\}_{i=1,...,N}$. Notice that q_i is associated with the box Ω_i and can also be associated with $x_{i-1/2}$.

The discretisation we use is based on the piecewise constant approximation of J_ψ, J_n and J_p on the dual mesh $\{D_i\}$. These piecewise constant functions are derived from q_h by

$$J_{\psi,i} = \lambda^2 \frac{\psi_{i+1} - \psi_i}{x_{i+1/2} - x_{1-1/2}}, \tag{3.1}$$

and

$$J_{n,i} = \mu_n \exp(\alpha\psi - \alpha\phi_n) \nabla(\alpha\phi_n) \qquad on D_i,$$

which yields

$$J_{n,i} = (\nabla\alpha\psi)\mu_n \frac{\exp(-\alpha\phi_n)|_{x_{i-1/2}}^{x_{i+1/2}}}{\exp(-\alpha\psi)|_{x_{i-1/2}}^{x_{i+1/2}}} = \tag{3.2}$$

$$= \mu_n \frac{\exp(-\alpha\phi_{n,i+1}) - \exp(-\alpha\phi_{n,i})}{\exp(-\alpha\psi_{i+1}) - \exp(-\alpha\psi_i)} \cdot \frac{\alpha\psi_{i+1} - \alpha\psi_i}{x_{i+1/2} - x_{i-1/2}}.$$

Similarly an expression is found for $J_{p,i}$,

$$J_{p,i} = \mu_p \frac{\exp(+\alpha\phi_{p,i+1}) - \exp(+\alpha\phi_{p,i})}{\exp(+\alpha\psi_{i+1}) - \exp(+\alpha\psi_i)} \cdot \frac{\alpha\psi_{i+1} - \alpha\psi_i}{x_{i+1/2} - x_{i-1/2}}. \tag{3.3}$$

Boundary conditions are treated in a way consistent with the assumption of piecewise constant J. In this way we obtain the discrete form of (2.6)

$$N_h(q_h) = r_h(q_h). \tag{3.4}$$

4. Nested discretisations

In fact, by the above construction we derived a cell-centered version of the well-known Scharfetter-Gummel scheme. What is important is the derivation of this scheme as a Galerkin or weighted residual method. We can define a residual weighting, or *restriction operator* $\bar{R}_h: V \to V_h$ by

$$\bar{R}_h u = u_h \tag{4.1}$$

where

$$(u_h)_i = \int\int_{\Omega_i} u(x)\, d\Omega, \qquad i = 1,2,...,N.$$

An interpolation or *prolongation operator* $P_h: S_h \to S$ is defined by the assumptions (i) that $(P_h q_h)(x_{i-1/2}) = q_i$, (ii) that $P_h q_h$ has piecewise constant fluxes J_ψ, J_n and J_p on the dual mesh $\{D_i\}$, and (iii) that $P_h q_h$ satisfies the boundary conditions for

(2.2) at x_0 and x_N. For (ψ,ϕ_n,ϕ_p) such that $P_h q_h = q = (\psi,\phi_n,\phi_p)$, this implies that q satisfies the boundary conditions, and that ψ is a piecewise linear function which interpolates the values $\{\psi_i\}_{i=1,\ldots,N}$. For ϕ_n and ϕ_p it leads to piecewise exponential interpolation, as is derived from (3.2). For $x \in D_i$ we find

$$\frac{\exp(-\alpha\phi_n)|_{x_{i-1/2}}^{x}}{\exp(-\alpha\psi)|_{x_{i-1/2}}^{x}} = \frac{\exp(-\alpha\phi_n)|_{x_{i-1/2}}^{x_{i+1/2}}}{\exp(-\alpha\psi)|_{x_{i-1/2}}^{x_{i+1/2}}}, \tag{4.2.a}$$

and

$$\exp(-\alpha\phi_n(x)) - \exp(-\alpha\phi_{n,i}) = \tag{4.2.b}$$
$$= (\exp(-\alpha\psi(x)) - \exp(-\alpha\psi_i)) \cdot \frac{\exp(-\alpha\phi_{n,i+1}) - \exp(-\alpha\phi_{n,i})}{\exp(-\alpha\psi_{i+1}) - \exp(-\alpha\psi_i)}.$$

This formula gives a kind of exponential interpolation formula for $\phi_n(x)$, interpolating the values $\{\phi_{n,i}\}_{i=1,\ldots,N-1}$. A similar formula is found for ϕ_p:

$$\exp(\alpha\phi_p(x)) - \exp(\alpha\phi_{p,i}) = \tag{4.2.c}$$
$$= (\exp(\alpha\psi(x)) - \exp(\alpha\psi_i)) \cdot \frac{\exp(\alpha\phi_{p,i+1}) - \exp(\alpha\phi_{p,i})}{\exp(\alpha\psi_{i+1}) - \exp(\alpha\psi_i)}.$$

In this way, the discrete operator $N_h q_h$ is constructed as the Galerkin operator $N_h = \bar{R}_h N(P_h q_h)$. Notice that the complete discretisation of $(N_h - r_h)$ is not a true Galerkin approximation because of the quadrature approximation used to compute r_h, the discrete version of the rhs in (2.5.a).

Given Ω_H, a discretisation of Ω, we can construct a sequence of finer and finer discretisations by successively doubling the number of boxes. Thus, we obtain $\Omega_{H/2}$, $\Omega_{H/4}$ etc.. In these discretisations all *boxes are nested,* i.e. a single box on a coarser discretisation contains a number of complete boxes in a finer discretisation. Notice that the corresponding dual boxes are *not* nested.

For each discretisation Ω_h in the sequence, we have spaces S_h, V_h and operators P_h, $\bar{R}_h$, N_h and r_h. Based on (4.1), a restriction operator $\bar{R}_{2h,h}: V_h \to V_{2h}$ can be introduced by

$$(\bar{R}_{2h,h} v_h)_i = \sum_{\Omega_{h,j} \subset \Omega_{2h,i}} v_{h,j}, \tag{4.3}$$

which satisfies the relation $\bar{R}_{2h,h} \bar{R}_h = \bar{R}_{2h}$.
Because the dual boxes are not nested, we can not find a prolongation $P_{h,2h} : S_{2h} \to S_h$ that satisfies the similar relation $P_{2h} = P_h P_{h,2h}$. Nevertheless we can construct a $P_{h,2h}$ such that

$$\bar{R}_{2h,h} N_h (P_{h,2h} q_{2h}) = N_{2h}(q_{2h}) \tag{4.4}$$

for all $q_{2h} \in S_{2h}$, by using for $P_{h,2h}$ interpolation rules derived from (4.2).

5. The Multigrid Method

To solve the nonlinear system

$$M_h(q_h) := N_h(q_h) - r_h(q_h) = f_h \tag{5.1}$$

we use a nonlinear multigrid (FAS) method [1, 2] . For a vanishing right-hand-side f_h this system is the system of equations (3.4). The FAS method for solving (5.1) is an iterative process, in which each cycle consists of:

1. a number of p nonlinear relaxation sweeps;
2. a coarse grid correction;
3. another q nonlinear relaxation sweeps.

As a *relaxation* procedure we use a nonlinear Collective Symmetric Gauss Seidel (CSGS) relaxation. In this procedure all boxes are successively scanned in forward and backward direction, and for each box in its turn the 3 nonlinear equations are (approximately) solved. The *coarse grid correction* consists of the following steps

$$d_{2h} = \bar{R}_{2h,h}(f_h - M_h(q_h^{(n)})), \tag{5.2.a}$$

$$M_{2h}(\tilde{q}_{2h}) = M_{2h}(q_{2h}) + d_{2h}/\mu, \tag{5.2.b}$$

$$q_h^{(n+1)} = q_h^{(n)} + \mu(P_{h,2h}\tilde{q}_{2h} - P_{h,2h}q_{2h}). \tag{5.2.c}$$

Here q_{2h} is an (arbitrary) approximation to the solution on the grid Ω_{2h}. The value $\tilde{q}_{2h}$ may be either computed from the nonlinear system (5.2.b), or it may be an approximated by a number of σ multigrid cycles for the solution of (5.2.b) applied to the initial approximation q_{2h}. In this way a recursive procedure is obtained in which a sequence of coarser and coarser grids is used. Only on the coarsest grid a (smaller) nonlinear system is to be solved by other means. The parameter $\mu \in \mathbb{R}$ is a number to control the right-hand-side in the equation (5.2.b). In our applications we use $\mu = 1$ throughout. The numbers $p, q, \sigma \in \mathbb{N}$ determine the *strategy* of the multigrid method; $\sigma = 1$ defines a V-cycle, $\sigma = 2$ a W-cycle. In most experiments we took a fixed strategy with $p = q = \sigma = 1$. The operators $\bar{R}_{2h,h}$ and $P_{h,2h}$ are as described in section 4.

There is a difference between the usual FAS algorithm and the present one, due to the nonlinearity of the prolongation. Generally, the last step in the coarse grid correction is written

$$q_h^{(n+1)} = q_h^{(n)} + \mu P_{h,2h}(\tilde{q}_{2h} - q_{2h})$$

which is equivalent to (5.2.c) only for a linear prolongation.

With the property $N_{2h} = \bar{R}_{2h,h}N_hP_{h,2h}$ it can be shown that the restriction of the residual will be small after a coarse grid correction. From (5.2.a-b), with M replaced by N we derive

$$\begin{aligned}\bar{R}_{2h,h}(f_h - N_h(q_h^{(n)})) &= \mu\,(N_{2h}(\tilde{q}_{2h}) - N_{2h}(q_{2h})) \\ &= \mu\,\bar{R}_{2h,h}N_h(P_{h,2h}\tilde{q}_{2h}) - \mu\,\bar{R}_{2h,h}N_h(P_{h,2h}q_{2h}),\end{aligned}$$

This implies for the restriction of the residual that

$$\bar{R}_{2h,h}(f_h - N_h(q_h^{(n+1)})) =$$

$$= \bar{R}_{2h,h}[N_h(q_h^{(n)}) - N_h(q_h^{(n+1)}) + \mu N_h(P_{h,2h}\tilde{q}_{2h}) - \mu N_h(P_{h,2h}q_h)].$$

Introducing the notation $\Delta q_h = q_h - q_h^*$, assuming that N_h is differentiable, and linearising N_h around q_h^*, we find

$$\begin{aligned}
&\bar{R}_{2h,h}(f_h - N_h(q_h^{(n+1)})) = \\
&= \bar{R}_{2h,h}[N_h' q_h^{(n)} - N_h' q_h^{(n+1)} + \mu N_h' P_{h,2h}\tilde{q}_{2h} - \mu N_h' P_{h,2h}q_{2h}] \\
&\quad + \mathcal{O}(\|\Delta q_h^{(n)}\|^2 + \|\Delta q_h^{(n+1)}\|^2 + \|\Delta P_{h,2h}\tilde{q}_{2h}\|^2 + \|\Delta P_{h,2h}q_{2h}\|^2) \\
&= \bar{R}_{2h,h} N_h'[q_h^{(n)} - q_h^{(n+1)} + \mu(P_{h,2h}\tilde{q}_{2h} - P_{h,2h}q_h)] \\
&\quad + \mathcal{O}(\|\Delta q_h^{(n)}\|^2 + \|\Delta q_h^{(n+1)}\|^2 + \|\Delta P_{h,2h}q_{2h}\|^2 + \|\Delta P_{h,2h}\tilde{q}_{2h}\|^2) \\
&= \mathcal{O}(\|\Delta q_h^{(n)}\|^2 + \|\Delta q_h^{(n+1)}\|^2 + \|\Delta P_{h,2h}q_{2h}\|^2 + \|\Delta P_{h,2h}\tilde{q}_{2h}\|^2).
\end{aligned}$$

For nonvanishing r_h, r_{2h} we obtain

$$\begin{aligned}
&\bar{R}_{2h,h}(f_h - M_h(q_h^{(n+1)})) = \\
&= \mu[r_{2h}(q_{2h}) - r_{2h}(\tilde{q}_{2h})] + \bar{R}_{2h,h}[r_h(q_h^{(n+1)}) - r_h(q_h^{(n)})] + \mathcal{O}(\|\,.\,\|^2) \\
&= \mu r'_{2h}(q_{2h} - \tilde{q}_{2h}) + \bar{R}_{2h,h} r'_h(q_h^{(n+1)} - q_h^{(n)}) + \mathcal{O}(\|\,.\,\|^2) \\
&= \mu[r'_{2h}(q_{2h} - \tilde{q}_{2h}) - \bar{R}_{2h,h} r'_h(P_{h,2h}q_{2h} - P_{h,2h}\tilde{q}_{2h})] + \mathcal{O}(\|\,.\,\|^2),
\end{aligned}$$

where we assume that r_h and r_{2h} are differentiable in a sufficient neighbourhood of q_h^* and q_{2h}^*. Using the differentiability of $P_{h,2h}$, we find

$$\begin{aligned}
\bar{R}_{2h,h}(f_h - M_h(q_h^{(n+1)})) &= \mu[\bar{R}_{2h,h}r'_h P'_{h,2h} - r'_{2h}](\tilde{q}_{2h} - q_{2h}) \\
&\quad + \mathcal{O}(\|\Delta q_h^{(n)}\|^2 + \|\Delta q_h^{(n+1)}\|^2 + \|\Delta P_{h,2h}q_{2h}\|^2 + \|\Delta P_{h,2h}\tilde{q}_{2h}\|^2).
\end{aligned}$$

We see that the restriction of the residual,

$$\bar{R}_{2h,h}(f_h - M_h(q_h^{(n+1)})) \approx (\bar{R}_{2h,h}r'_h P'_{h,2h} - r'_{2h})(\tilde{q}_{2h} - q_{2h}),$$

depends on the integration error in the right-hand-side, which will be at most $\mathcal{O}(h)$. In general $\tilde{q}_{2h} - q_{2h}$ will be at most $\mathcal{O}(h)$, and the restriction of the residual will be $\mathcal{O}(h^2)$.

Because $\bar{R}_{2h,h}$ adds residual components of small boxes to form a residual component of a coarse grid box, a small value of $\bar{R}_{2h,h}(f_h - M_h(q_h^{(n+1)}))$ implies that large components in $f_h - M_h(q_h^{(n+1)})$ must be high-frequency components. The success of the MG method is based on the fact that relaxation methods as CSGS are effective means to reduce these high frequency components in the error/residual.

In principle, for the smoothing step we may consider various relaxations. Based on previous experience with other equations, our choice is Collective Symmetric Gauss Seidel relaxation. This relaxation can be performed in different ways. In all cases the boxes are successively scanned, first in the forward later in the backward direction, and in each box in its turn the 3 nonlinear equations are approximately solved. How the solution of these small systems is approximated makes the difference. The first possibility is to use Newtons method. Another possibility is pointwise Gummel iteration. In Gummel iteration, first the variable ψ is solved for fixed values of ϕ_n and ϕ_p, and then ϕ_n and ϕ_p are solved for the new value of ψ. In

pointwise Gummel relaxation, this process is iterated for each particular cell until the solution of the nonlinear 3×3 system is obtained with a specified accuracy.

At convergence, the result of this pointwise iteration process and the result of pointwise Newton iteration are the same. Differences are the faster convergence of the Newton process near the solution, and the better global convergence properties of the pointwise Gummel iteration. An additional advantage of Gummel iteration is that no (possibly ill conditioned) linear 3×3 systems have to be solved.

6. The test problem

As a test problem we consider a simple one-dimensional standard diode as described in[3] . It is given by the equation (2.2) in one space dimension, on the interval (0.0,0.001); with $\epsilon = 1.0359\text{E}-12$, $q = 1.6021\text{E}-19$, $n_i = 1.22\text{E}+10$, $\alpha = 38.68293$. The dope function is given by

$$D(x) = \begin{cases} -1.0E\,18, & \text{if } x<0.0005\,, \\ +1.0E\,18, & \text{if } x>0.0005\,, \end{cases}$$

$R = 0$ and μ_n and μ_p are constants.
At the boundary charge neutrality is required: $p - n + D = 0$. Further, at $x = 0$ the boundary conditions are $\phi_n = \phi_p = 0$; at $x = 0.001$ the applied voltage v_B is given $\phi_n = \phi_p = v_B$.

Computations have been made for $v_B = 5.0$ (the standard case) and further for $v_B = 100.0$ (reverse bias) and $v_B = -1.0$ (forward bias).

For the discretisation two kinds of mesh are used: (1) a uniform, and (2) a non-uniform mesh. Both meshes were used with $N = 2^L$, $L = 0,1,\cdots,8$ cells. The non-uniform mesh was defined by the mapping $x_i = f(\xi_i)$, where f is a differentiable and monotonously increasing function, and $\{\xi_i\}_{i=0,\cdots,N}$ a uniform partition of [0,1]. This function f is chosen such that a reasonable resolution of the layer at $x = 0.0005$ can be obtained. At first sight it seems unreasonable to try uniform meshes for these problems, because it is known that the solution is rapidly varying near the depletion layer. Nevertheless, we are also interested in the behaviour of the numerical methods for this case, because we want to know how the numerical methods behave for not well-adapted coarse meshes.

Results and conclusion.

We find that, for a 1-D diode as model problem, typical multigrid convergence can be obtained for the discrete semiconductor device equations. A convergence factor is found that is essentially independent of the meshwidth. By embedding in a "Full Multigrid" algorithm, one or two iteration steps seem to be sufficient to reduce the iteration error below truncation error. For this purpose, in the non-linear FAS-procedure the prolongation was adapted to the method of discretisation (Scharfetter-Gummel). It appeared that discrete operators on extremely coarse meshes still enhance the convergence behaviour.
A more detailed description of the method and the results will be published later.

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