Numerical Analysis of Semiconductor Devices

John Carroll

1 Introduction

Although the device modeling problem is perhaps one of the most difficult computational problems in current research, there is a dramatic increase in reliance on process and device simulation tools for technology development and device optimization. The characteristic feature of early modeling was the separation of the interior into different regions, whose treatment could be simplified by various assumptions like special doping profiles, completion regions and quasi-neutrality. These separately treated regions were simply connected to produce the overall solution.

Fully numerical device modeling based on partial differential equations which describe all different regions of semiconductor devices in a single unified manner was first suggested by Gummel [11] for the one-dimensional bipolar transistor. This approach was further developed and applied to pn-junction theory by De Mari [7] and to IMPATT diodes by Sharfetter and Gummel [15]. A two-dimensional numerical analysis of a semiconductor device was first undertaken by Kennedy and O'Brien [12] who investigated the junction field effect transistor. Since then, two-dimensional modeling has been applied to almost all important semiconductor devices.

It is now universally accepted that device simulation tools provide a worthwhile alternative to the conventional experimental approach of running wafer lots through a process line. We present a brief overview of the numerical techniques which are being employed to solve the coupled system of highly nonlinear partial differential equations which model the behaviour of electron and holes in a semiconductor structure. We begin in Section 2 with an introduction to the basic semiconductor equations in order to define the relevant physical variables. The scaling procedures and dependent variable alternatives are considered briefly in Section 3 while Section 4 concentrates mainly on the discrete form of the mathematical equations. The nonlinear and linear solution strategies as well as certain algorithmic factors are discussed in Section 5.

2 The Semiconductor Equations

The partial differential equations which model the steady-state and transient behaviour of carriers under the influence of external fields can be derived, in a semiclassical framework, from the Boltzmann Transport Equation. In this way, carrier motion is considered as a series of acceleration events (described by classical mechanics) and scattering events (described by quantum mechanics). If we assume that the response of carriers to a change in the electric field is considerably faster than the rate of change of the field itself, we can write the basic equations of semiconductor transport in the most commonly used form [16] as follows.

The Poisson equation

$$\epsilon_s \nabla \cdot \mathbf{E} = -\epsilon_s \nabla^2 \psi = \rho \tag{1}$$

relates the total space charge ρ to the divergence of the electric field $\mathbf{E}$, which defines the electrostatic potential ψ as

$$\mathbf{E} = -\nabla \psi \tag{2}$$

Under the assumption of total ionization, the total space charge ρ is given as

$$\rho = -q(n - p + \Gamma) \tag{3}$$

where $\Gamma = N_D^+ - N_A^-$ is the total electrically active net impurity concentration, q is the electric charge, and n and p are the electron and hole densities respectively. The connection between the behaviour of the carrier densities and the electric field is given by the current equations for electrons and holes

$$\mathbf{J}_n = q\mu_n n\mathbf{E} - qD_n \nabla n \tag{4}$$

$$\mathbf{J}_p = q\mu_p p\mathbf{E} + qD_p \nabla p \tag{5}$$

where μ_n and μ_p are the electron and hole mobilities and D_n and D_p are the corresponding diffusion coefficients. Both mobilities and diffusion coefficients depend on the temperature, the doping level and the electric field.

The electron and hole concentrations may be written as

$$n = n_{ie} \exp \frac{q(\psi - \phi_n)}{kT} \tag{6}$$

$$p = n_{ie} \exp \frac{q(\phi_p - \psi)}{kT} \tag{7}$$

where we have defined the *quasi-Fermi potentials* ϕ_n and ϕ_p [16]. The factor n_{ie} is the effective carrier concentration. For low doping, n_{ie} approaches the intrinsic carrier concentration n_i. If we assume the *Einstein relation* [17] for both electrons and holes

$$D = \mu \frac{kT}{q} \tag{8}$$

then equations (4) and (5) can be re-written using (6) and (7) as

$$\mathrm{J}_n = q\mu_n n \nabla \phi_n \tag{9}$$

$$\mathrm{J}_p = q\mu_p p \nabla \phi_p \tag{10}$$

The continuity equations for electrons and holes are given by

$$\frac{\partial n}{\partial t} = -\frac{1}{q}\nabla \cdot \mathrm{J}_n - R + G \tag{11}$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\nabla \cdot \mathrm{J}_p - R + G \tag{12}$$

where G and R represent generation and recombination processes respectively. In some applications, generation is ignored and the Shockley-Read-Hall steady state recombination is adopted, namely

$$R = \frac{pn - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)} \tag{13}$$

where τ_n and τ_p are respectively the electron and hole lifetimes.

In the time dependent case, the equation of total current continuity couples the change in electric field strength to the current densities

$$\nabla \cdot \mathrm{J}_T = \nabla \cdot \left(\epsilon \frac{\partial \mathrm{E}}{\partial t} + \mathrm{J}_n + \mathrm{J}_p \right) \tag{14}$$

where J_T is the total current, which consists of both the conduction components J_n and J_p and the displacement current $\epsilon\, \partial \mathrm{E}/\partial t$.

The boundary conditions for semiconductor devices are given by neutrality and equilibrium conditions, namely

$$pn = n_i^2 \tag{15}$$

$$n - p + \Gamma = 0 \tag{16}$$

Thus at a Dirichlet contact, the three potentials are

$$\psi = V_c(t) + V_{bi} \tag{17}$$

$$\phi_n = \phi_p = V_c(t) \tag{18}$$

where V_{bi} and $V_c(t)$ are the built-in and contact voltages respectively. When external circuit elements are applied to the device, the contact voltage becomes an unknown and is given by

$$\frac{1}{R}[V_c(t) - V_a(t) + C\frac{d}{dt}[V_c(t) - V_a(t)] + \int_\Gamma \nabla \cdot \mathrm{J}\, dl = 0 \tag{19}$$

where R, C and $V_a(t)$ are the resistance, capacitance and applied voltage respectively and Γ is an appropriate contour surrounding the contact.

The complete set of semiconductor equations is given by (1), (9), (10), (11) and (12) together with appropriate initial and boundary conditions and, as we will see in the next section, this set of coupled nonlinear partial differential equations are usually written in dimensionless form appropriate for numerical simulation.

3 Problem Formulation

Before proceeding to the numerical solution, there are a number of factors which must be considered, notably the choice of dependent variables and an appropriate scaling of the equations. The choice of variables can crucially affect the linearity of the equations as well as the symmetry of the iteration matrix. Scaling is important as the dependent variables can be of different order of magnitudes and show a strongly different behaviour in regions with small and large space charge.

For the system with dependent variables $\{\psi, n, p\}$, a standard approach to scaling was proposed by de Mari, see [8], where ψ is scaled by the thermal voltage $V_t = \frac{kT}{q}$; n and p are scaled by n_i and the independent variables are scaled such that all multiplying constants in Poisson's equation become unity — all spatial quantities are scaled by the intrinsic *Debye* length $L_i = \sqrt{\epsilon_s kT/qn_i}$. This approach may be physically reasonable but suffers in that the variables n and p are still several orders of magnitude larger than ψ. An alternative "singular perturbation approach" was proposed in [1] which effectively reduces the variables ψ, n and p to the same order of magnitude. In this case, the variables n and p are scaled by the maximum absolute value of the net doping Γ and the independent variables are scaled by the characteristic length of the device.

Following [8] for example, the basic equations can be written in normalized form as

$$\begin{aligned} g_1(\psi, n, p) &= -\nabla^2\psi + n - p - k_1 = 0 \\ g_2(\psi, n, p) &= \frac{\partial n}{\partial t} + \nabla \cdot J_n + k_2 = 0 \\ g_3(\psi, n, p) &= \frac{\partial p}{\partial t} - \nabla \cdot J_p + k_2 = 0 \end{aligned} \tag{20}$$

where ψ, n, p, J_n and J_p are the normalized electrostatic potential, carrier densities and current densities respectively, and k_1 and k_2 represent the normalized impurity concentration and generation-recombination terms. We could also write the system in terms of the normalized quasi-Fermi potentials ϕ_n and ϕ_p as follows:

$$\begin{aligned} g_1(\psi, \phi_n, \phi_p) &= -\nabla^2\psi + e^{\psi-\phi_n} - e^{\phi_p-\psi} - k_1 = 0 \\ g_2(\psi, \phi_n, \phi_p) &= \frac{\partial e^{\psi-\phi_n}}{\partial t} + \nabla \cdot (\mu_n e^{\psi-\phi_n} \nabla\phi_n) + k_2 = 0 \\ g_3(\psi, \phi_n, \phi_p) &= \frac{\partial e^{\phi_p-\psi}}{\partial t} - \nabla \cdot (\mu_p e^{\phi_p-\psi} \nabla\phi_p) + k_2 = 0 \end{aligned} \tag{21}$$

There are many choices for the set of dependent variables and, in what follows, we will refer to the arbitrary choice u, v, w as including such possibilities as $\{\psi, n, p\}$, $\{\psi, \phi_n, \phi_p\}$, $\{\psi, \psi-\phi_n, \psi-\phi_p\}$ or perhaps $\{\psi, \Phi_n, \Phi_p\}$ where $\Phi_n = e^{-\phi_n}$ and $\Phi_p = e^{\phi_p}$ all of which have appeared in recent publications. The first set of variables used in device simulation was the potential and carrier concentrations but, because the continuity matrix took on a positive definite

form, many workers switched to exponentials of the quasi-Fermi potentials. The quasi-Fermi potentials themselves are now quite popular and offer the advantage of reducing the numerical range of the dependent variables.

4 Discretization

Software for device analysis could roughly be classified in two categories. One of these involves codes for analysis of specified device types. These codes often utilize a regular mesh, finite difference discretization and iterative solution methods. Since the device type is known, some behaviour of the structure can be predicted. This information can be used to select appropriate physical parameters and to improve the mesh generation and the equation solution methods. The second category contains codes for analysis of an arbitrary semiconductor structure. They are characterized by a high degree of flexibility which makes the user more responsible for the final results. The finite element method (fem) has many properties which motivate its usage in this category.

As an illustration, we will consider the steady state case, i.e. where $\frac{\partial n}{\partial t} = \frac{\partial p}{\partial t} = 0$ with exponentials of the quasi-Fermi levels, $\Phi_n = \exp(-\phi_n)$ and $\Phi_p = \exp(\phi_p)$, as dependent variables. Ignoring the generation term, we consider the one-dimensional form

$$\begin{aligned} -\frac{d^2\psi}{dx^2} &= \Phi_p e^{-\psi} - \Phi_n e^{\psi} + \Gamma(x) \\ \frac{dJ_p}{dx} &= R \\ \frac{dJ_n}{dx} &= -R \end{aligned} \tag{22}$$

where

$$J_p = \frac{d\Phi_p}{dx} e^{-\psi}$$

$$J_n = -\frac{d\Phi_n}{dx} e^{\psi}$$

A constant space charge density results in a parabolic function for ψ and we therefore use a standard Taylor's expansion to discretize (22). First we define the non-uniform mesh on $[0, 1]$

$$x_0 = 0$$

$$x_{j+1} = x_j + h_j, 0 \leq j \leq N-1$$
$$x_N = 1$$

where the h_j are suitably chosen to model rapidly varying solution behaviour and are typically constrained by the inequality

$$\max_j\left(\frac{h_{j+1}}{h_j}, \frac{h_j}{h_{j+1}}\right) \leq 2$$

for all $0 \leq j \leq N-1$. Before linearization, the difference scheme corresponding to Poisson's equation has the form

$$-D_+D_-\psi_j = \Phi_{p,j}e^{-\psi_j} - \Phi_{n,j}e^{\psi_j} + \Gamma_j \tag{23}$$

where the difference operator D_+D_- is the standard three-point difference operator on a non-uniform mesh

$$D_+D_-y_i = \frac{2}{h_ih_{i-1}(h_i+h_{i-1})}[h_iy_{i-1} - (h_i+h_{i-1})y_i + h_{i-1}y_{i+1}]$$

The standard Taylor expansion has proved inadequate however for the continuity equations since this approach, for the quasi-Fermi potentials for example, would suggest exponential current density profiles. In reality current densities are known not to vary very rapidly with respect to the spatial coordinate. Hence we employ the Sharfetter-Gummel discretization (see [15]) which incorporates approximate integrals of the basic equations into the formulation of the difference equations and yields constant current densities between adjacent mesh points. Taking the hole current for example and recalling that

$$\frac{d\Phi_p}{dx} = J_pe^{\psi}$$

we integrate over the interval $[x_j, x_{j+1}]$ on which we assume that the current density is constant and that the electrostatic potential is linear. Thus we get

$$\begin{aligned}\Phi_{p,j+1} - \Phi_{p,j} &= \int_{x_j}^{x_{j+1}} J_pe^{\psi}\,dx \\ &= J_{p,j+\frac{1}{2}}\int_{x_j}^{x_{j+1}} \frac{d(e^{\psi})}{\frac{d\psi}{dx}} \\ &= h_jJ_{p,j+\frac{1}{2}}\frac{e^{\psi_{j+1}} - e^{\psi_j}}{\psi_{j+1}-\psi_j}\end{aligned}$$

or equivalently we write

$$J_{p.j+\frac{1}{2}} = e^{-\psi_j}D_+\Phi_{p,j}B(\Delta\psi_j)$$

where we introduce the notation

$$D_+z_i = \frac{z_{i+1}-z_i}{h_i}$$
$$\Delta z_i = z_{i+1} - z_i$$
$$B(x) = \frac{x}{e^x - 1}$$

The corresponding difference expression over the interval $[x_{j-1}, x_j]$ may be found analogously. The current density approximations may be summarised as follows

$$J_{p,j+\frac{1}{2}} = e^{-\psi_j}B(\Delta\psi_j)D_+\Phi_{p,j} \tag{24}$$
$$J_{p,j-\frac{1}{2}} = e^{-\psi_j}B(-\Delta\psi_{j-1})D_+\Phi_{p,j-1} \tag{25}$$
$$J_{n,j+\frac{1}{2}} = -e^{\psi_j}B(-\Delta\psi_j)D_+\Phi_{n,j} \tag{26}$$
$$J_{n,j-\frac{1}{2}} = -e^{\psi_j}B(\Delta\psi_{j-1})D_+\Phi_{n,j-1} \tag{27}$$

Using a standard centered difference approximation, the continuity equations can be discretized as follows

$$\frac{2}{h_{j-1}+h_j}[J_{p,j+\frac{1}{2}} - J_{p,j-\frac{1}{2}}] = R_j \tag{28}$$
$$\frac{2}{h_{j-1}+h_j}[J_{n,j+\frac{1}{2}} - J_{n,j-\frac{1}{2}}] = -R_j \tag{29}$$

and, on using equations (24) to (27), these become

$$B(-\Delta\psi_{j-1})D_+\Phi_{p,j-1} - B(\Delta\psi_j)D_+\Phi_{p,j} = -\frac{(h_{j-1}-h_j)}{2}e^{\psi_j}R_j \tag{30}$$

$$B(\Delta\psi_{j-1})D_+\Phi_{n,j-1} - B(-\Delta\psi_j)D_+\Phi_{n,j} = -\frac{(h_{j-1}+h_j)}{2}e^{-\psi_j}R_j \tag{31}$$

The difference equations (23), (30) and (31), subject to appropriate boundary conditions provide the basis for the numerical solution procedures in one-dimensional steady state simulations.

Any discretization scheme for the semiconductor device equations should possess certain desirable properties. In particular, it should

- function in arbitrary geometries
- be conservative
- provide adequate treatment of drift-diffusion terms
- allow convenient enforcement of boundary and interface conditions
- permit adaptive mesh construction
- be free of dimensional restrictions

There are a number of discretization strategies in current use — the "finite difference method", of which the foregoing is an example, the "finite box method" which is just a more general finite difference method and the "finite element method". No attempt is made to provide a serious mathematical preference for one method or the other. The finite difference method and the finite element method are frequently considered to be mutually independent from the beginning. However it is often a matter of interpretation only and one can sometimes obtain the exact same discrete equations from either a finite difference approach or a finite element approach. It should be noted however that finite difference formulae accounting for normal derivatives at a curved boundary are extremely awkward so that, for this type of problem, one should consider the finite element method.

5 Numerical Solution Procedures

The exponential dependency of n and p on ψ makes Poisson's equation nonlinear and the generation-recombination mechanisms couple the two current continuity equations and introduce strong nonlinearities. There are basically two different solution strategies adopted for the discretized system namely (a) the decoupled (or Gummel) and (b) the coupled (or simultaneous) procedure. Both require an initial guess of the solution followed by an adjustment of the guess until an acceptable degree of accuracy is obtained.

5.1 The Decoupled Approach

This approach is sometimes referred to as the Gummel iteration [11] by electrical engineers and the Jacobi / Gauss-Seidel iteration by mathematicians

and treats the three equations independently. The iteration proceeds by associating with each g_i the highest-order differential dependent variable (e.g. for the variables of equation (20), taking ψ in the first equation and n and p in the other two respectively). In solving $g_1 = 0$, v and w are treated as fixed to obtain a new solution for u. Let $z_k = (u_k, v_k, w_k)^T$. The iteration can be written as

$$\begin{aligned} g_1(z_k \rightarrow u_{k+1}) &= 0 \\ g_2(z_k, u_{k+1} \rightarrow v_{k+1}) &= 0 \\ g_3(z_k, u_{k+1}, v_{k+1} \rightarrow w_{k+1}) &= 0 \end{aligned} \tag{32}$$

where the variables left of $\rightarrow$ are considered as input variables. This symbolic representation of the iteration allows considerable flexibility in determining the sequence of one-variable equations.

The partitioning of the complete PDE system into a series of three equations that can be solved independently made this procedure very popular particularly in the early years of device modeling. The applicability of the Gauss-Seidel approach however depends critically on the level of current flow inside the device structure. In [4] the procedure has been found to work very well for conditions of low to medium current flow and negligible generation-recombination terms k_2. This corresponds to a weak coupling of the PDE system where the density or quasi-Fermi potentials act as small perturbations to the Poisson equation.

5.2 The Coupled Approach

Using the Gauss-Seidel iteration in physical situations where there is heavy coupling between the variables (typically in high current conditions) will usually prove to be difficult and, in most cases, convergence will not be realised. As a result, reasearchers quickly turned to a more robust procedure based on Newton's method. This requires both the assembly and the approximate solution of the system

$$\frac{\partial g_k}{\partial z_k} x = -g_k \tag{33}$$

where $g_k = g(u_k, v_k, w_k)$ with $g = (g_1, g_2, g_3)^T$. In expanded form this leads to the system

$$\begin{pmatrix} \frac{\partial g_1}{\partial u} & \frac{\partial g_1}{\partial v} & \frac{\partial g_1}{\partial w} \\ \frac{\partial g_2}{\partial u} & \frac{\partial g_2}{\partial v} & \frac{\partial g_2}{\partial w} \\ \frac{\partial g_3}{\partial u} & \frac{\partial g_3}{\partial v} & \frac{\partial g_3}{\partial w} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = - \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix} \tag{34}$$

where the Jacobian matrix $\frac{\partial g}{\partial z}$ and the right hand side are evaluated at the k-th iteration (u_k, v_k, w_k). Unlike the decoupled algorithm, the simultaneous or coupled approach has the advantage that it is practically independent of the applied bias conditions and injection levels in the device. If the linear algebra modules are subsequently carefully chosen, it also proves to be sufficiently robust for general purpose codes. However, it suffers somewhat because of the increased requirements of CPU-performance and memory and, in this context, the use of approximate Newton methods are becoming more popular in an attempt to offset these factors.

5.3 Algorithmic Aspects

Assuming we wish to solve the nonlinear system of type (20) or (21) for example. Firstly, the large sparse linearized system

$$M_k x_k = -g(z_k) \equiv -g_k \tag{35}$$

is solved by the sparse direct or iterative methods (to be described) where M_k is an approximation to the exact Jacobian $\frac{\partial g}{\partial z}$. The next iterate is taken as

$$z_{k+1} = z_k + t_k x_k \tag{36}$$

where $t_k \in (0, 1]$ is chosen to satisfy the sufficient-decrease condition

$$1 - \frac{\| g_{k+1} \|}{\| g_k \|} > \epsilon\, t_k \tag{37}$$

and ϵ is the machine epsilon. In other words, the step-length parameter t_k damps the step x_k to insure that $\| g_{k+1} \| < \| g_k \|$ increasing the robustness of the nonlinear equation algorithm [3]. Moreover, t_k is biased towards unity so that a traditionally quadratically convergent method is recovered in the Newton-attraction region.

A popular Newton iterative method is the Newton-Richardson algorithm [4] which assumes that g_k can be written as

$$g_k = M_k - N_k \tag{38}$$

with

$$\| M_k^{-1} N_k \| = \| I - M_k^{-1} g_k \| \leq \rho_0 < 1 \tag{39}$$

for all k. In this case, M_k represents a previously factored Jacobian so that the method clearly attempts to exploit the fact that the time to factor a sparse matrix is much larger than the CPU time to perform a backsolve with a previously factored matrix. The x_k is found by an inner iteration

$$M_k(x_{k,l} - x_{k,l-1}) = -(\frac{\partial g_k}{\partial z_k} x_{k,l-1} + g_k) \tag{40}$$

where $x_{k,0} = 0$ and $x_k = x_{k,l_k}$ for some l_k. This inner iteration can be controlled by monitoring the quantities

$$\alpha_{k,l} = \frac{\| g_k + \frac{\partial g_k}{\partial x_k} x_{k,l} \|}{\| g_k \|} \tag{41}$$

Note that both quantities used to compute $\alpha_{k,l}$ are already available. The inner iteration is terminated when

$$\alpha_{k,l_k} \leq \alpha_0 \left(\frac{\| g_k \|}{\| g_0 \|} \right) \tag{42}$$

where $\alpha_0 \in (0, 1)$ is an experimentally determined parameter. We refer the interested reader to [3] for further details where it is shown that the resulting procedure is quadratically convergent.

5.4 Linear Equation Solution

The set of linear equations which must be solved at each iteration of the Newton procedure (outer iteration) is large and sparse. It may be symmetric or unsymmetric depending on the choice of dependent variables. The efficient solution of systems of linear equations is the key to any successful device simulator where typically the solution of a system of 6000 equations may be required. In terms of CPU and memory, the linear algebra portion of the

overall solution process dominates. Iterative techniques are usually preferred since they can fully exploit the sparsity of the equation set. Equally important, they can exploit the fact that the linear equations are part of the outer loop and only need to be solved sufficiently accurately to ensure that the outer loop converges rapidly.

In simulating an arbitrarily shaped structure, the box integration technique is often used with the finite difference method. Using this method, the solution of Poisson's equation and the current continuity equations can be reduced to the solution of linear systems of equations involving symmetric band matrices. The symmetry of the coefficient matrix not only saves memory but also enables the application of the highly popular ICCG (Incomplete Cholesky-decomposition and Conjugate gradient) [13] method which results in a very high speed simulation.

For unsymmetric matrices, both preconditioned ORTHOMIN [2] and preconditioned conjugate gradient squared have been studied with the latter showing a slight advantage. The conjugate gradient iteration (inner iteration) is continued until the norm monitored in the outer loop has decreased and the residuals of the preconditioned equation set has been reduced by a factor of typically 10^3.

To obtain the required convergence whilst exploiting the sparse structure, the choice of preconditioner is critical. The preconditioner employed relies heavily on the method in which the equations are ordered. To ensure that the coupling between the three equations is taken into account, the equations and variables associated with a given node are ordered sequentially. In this way, the coupling between the equations is represented by 3 by 3 submatrices distributed within the matrix. In addition, the nodes are ordered in a way that nodes with strong coupling are neighbours — this is achieved by numbering the nodes sequentially along a path through the mesh that always advances by moving to the closest node which is not yet ordered. Thus strong coupling of nodes is assumed to be correlated with a close spacing of the nodes. With this ordering of the equations, the matrix describing the set of linear equations is dominated by the components in the 3 central diagonals of 3 by 3 submatrices. An exact inverse of this "tridiagonal block" structure can be economically calculated and used to precondition the linear system.

6 Conclusion

We have attempted to provide a simple overview of some of the techniques and issues which are involved in the numerical analysis of semiconductor devices. During the last several years, the modeling of basic semiconductor device structures has grown in importance as integrated circuit complexity has increased. To reduce risk and enable aggressive circuit design, efficient and accurate compact models are required for the simulation of circuits containing hundreds and thousands of devices. These compact models must be fully characterized for the target fabrication process and be valid over a wide range of operating conditions including temperature variations. The predictive capabilities of detailed numerical device and process simulators can be used to enhance device characterization techniques and to form a basis for technology optimization.

Simulators that can perform DC-analysis of specific device types in two space dimensions are today in use at many process development facilities and this level may be considered state of the art. With a reduction in the geometrical dimensions of, for example, the MOSFET, there is an increasing necessity for three-dimensional device simulators and current research is rapidly providing the building blocks. In addition to three-dimensional device analysis, the simulator must also be capable of (a) treating irregularly shaped structures; (b) one- and two-dimensional simulations and (c) device parameter calculations. Two three-dimensional simulators in current use are FIELDAY [5] and TRANAL [18], both of whom first appeared in 1980 and, since then, attention has been focused on reducing the large memory capacity and computing time required for the simulation.

References

[1] Agler W., Markowich P.A., Selberherr S., *A singular perturbation analysis of discretization methods for the parabolic semiconductor equations*, Proceedings of the NASECODE III Conference, J. Miller (Ed.), Boole Press, Dublin 1983.

[2] Axelsson O., *Conjugate gradient type methods for unsymmetric systems of linear equations*, Linear Algebra and its Applics. **29** (1980).

[3] Bank R.E., Rose D.J., *Parameter selection for Newton-like methods applicable for nonlinear partial differential equations*, SIAM J. Numer. Anal. 17 (1980), 806–822.

[4] Bank R.E., Coughran W.M., Fichtner W., Grosse E.H., Rose D.J., Smith R.K., *Transient simulation of silicon devices and circuits*, IEEE Trans Electron Devices, ED-32 (1985), 1092–2007.

[5] Buturla E.M., Cottrell P.E., Grossman B.M., Salsburg K.A., *Finite-element analysis of semiconductor devices: the FIELDAY program* , IBM J. Res. Dev. 25 (1981), 218–231.

[6] Carroll J., *A one dimensional numerical model of the NPN transistor under arbitrary conditions*, Proceedings of the NASECODE IV Conference, J. Miller (Ed.), Boole Press, Dublin 1985.

[7] De Mari, *An accurate numerical steady state one-dimensional solution of the pn-junction*, Solid-State Electron 11 (1968), 35–58.

[8] De Mari, *An accurate numerical one-dimensional solution of the pn-junction under arbitrary transient conditions*, Solid-State Electron 11 (1968), 1021–1053.

[9] Fichtner W., Rose D.J. (Eds), *Special Issue on Numerical Modeling of VLSI Devices* , IEEE Trans Electron Devices, ED-30 (1983) Number 9.

[10] Fichtner W., Rose D.J. (Eds), *Special Issue on Numerical Modeling of VLSI Devices* , IEEE Trans Electron Devices, ED-32 (1985) Number 10.

[11] Gummel H.K., *A self consistent iterative scheme for one-dimensional steady state transistor calculations*, IEEE Trans. ED-11 (1964), 455–465.

[12] Kennedy D.P., O'Brien R.R., *Two dimensional mathematical analysis of a planar type junction field effect transistor*, IBM J. Res. Dev. 13 (1969), 662–674.

[13] Meijerink J.A., van der Vorst H.A., *An iterative solution method for linear systems of which the coefficient is a symmetric M-matrix* , Math. Comput. 31 (1977), 148–162.

[14] Mock M.S., *Analysis of Mathematical Models of Semiconductor Devices*, Boole Press, Dublin 1983.

[15] Sharfetter D.L., Gummel H.K., *Large-signal analysis of a Silicon-Read diode oscillator*, IEEE Trans Electron Devices ED-16 (1969), 64–77.

[16] Shockley W., *Electrons and Holes in Semiconductor Devices*, van Nostrum, Princeton 1950.

[17] Smith R.A., *Semiconductors*, Cambridge University Press, New York 1978.

[18] Yoshii A., Kitazawa H., Tomiyama M., Horiguchi S., Sudo T., *A three-dimensional analysis of semiconductor devices*, IEEE Trans Electron Devices, ED-29 (1982), 184–189.

Department of Mathematics
Dublin City University