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Nonlinear Block Iterative Solution of Semiconductor Device Equations by a Domain Decomposition Method[1]

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Abstract

A block nonlinear Gauss-Seidel procedure is employed to decouple the full system arising from the finite element approximation of the steady-state semiconductor device equations. At each iteration, a Neumann-Neumann domain decomposition method is applied to solve the linearized equations yielding electric potential and free carrier densities. Numerical results for one dimensional realistic test problems are given.

1 Introduction

The aim of this paper is to study a typical test device in semiconductor modeling, namely, a one-dimensional p-n diode. In section 2 we introduce the well-known *drift-diffusion* equations (see, e.g., [4]) that describe charge flow in a semiconductor device at steady-state conditions. The mathematical problem consists of a set of three highly nonlinearly coupled equations in the unknowns (ψ, n, p), which are respectively electric potential and carrier concentrations (electrons and holes). In order to reduce the computational effort, a block nonlinear Gauss-Seidel algorithm known in semiconductor literature as Gummel's map [3] is considered in section 3 to decouple the full system. The three resulting linearized equations are suitably formulated and then successively solved by a Neumann-Neumann domain decomposition method [1]. Concerning the spatial discretization, we respectively employ piecewise linear and exponentially fitted (*à la* Scharfetter-Gummel [7]) finite elements to handle the electric potential equation and the convection-diffusion equations for both electron and hole densities (see also [2] and [6]). In the concluding section 4 we discuss several numerical results relative to the study of the p-n diode at some working conditions of noteworthy interest.

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2 The drift-diffusion model for semiconductors

Steady-state charge flow throughout a semiconductor device in the one dimensional case is commonly modeled by the following elliptic boundary value problem (see, e.g., [4])

$$(1) \quad -\psi'' = \rho \qquad (4) \quad \rho = \rho(\psi, n, p) = (p - n + C)$$

$$(2) \quad \mathrm{J}'_n = R(\psi, n, p) \qquad (5) \quad \mathrm{J}_n = \mu_n(n' - n\psi')$$

$$(3) \quad \mathrm{J}'_p = -R(\psi, n, p) \qquad (6) \quad \mathrm{J}_p = -\mu_p(p' + p\psi')$$

The equations above represent the *drift-diffusion* model for a one dimensional semiconductor device and can be solved in any open set $\Omega = (0, L)$ provided by suitable boundary conditions.The unknowns (ψ, n, p) are respectively electric potential and free carrier densities (electrons and holes), so that (1) is a Poisson equation and (2)-(3) are two continuity equations for electron and hole current densities J_n and J_p. These latter are, for a given electric field $\mathrm{E} = -\psi'$, convection-diffusion equations with a (possibly) highly dominating transport in thin regions across the so called *p-n junctions*. The functions $\rho(x)$, $C(x)$, $\mu_{n,p}$, and R are respectively the space charge density, the doping profile, the carrier mobilities, and the net recombination/generation rate. For more details on the physical model, see [4] and the references therein.
Maxwell-Boltzmann statistics is assumed to hold, and therefore

$$(7) \quad n = \rho_n e^{\psi} \qquad (8) \quad p = \rho_p e^{-\psi}$$

where $\rho_{n,p}$ are usually known as *Slotboom* variables [8].

The choice of such a model problem makes the algorithmic effort relatively easy while retaining a wide range of generality, since the basic physical properties of the solutions in more complex and realistic geometries are well reproduced by the one dimensional approximation. A more detailed description of the mathematical model in the two dimensional case and of the numerical aspects is given in [4] and [5].

3 The solution algorithm

When facing the numerical approximation of (1)-(3), the most critical aspects are:

- the need of finding an effective linearization procedure that allows the decoupling of the three equations;
- the presence of sharp interior layers that demands use of domain decomposition methods and upwind finite elements.

On the ground of the numerical experiments performed, we propose the following solution algorithm, which is long established in semiconductor device

modeling and is commonly known as *Gummel's map* [3]. It reduces the overall computational effort by forcing a decoupling in system (1)-(3) and leading to the successive solution of one *nonlinear* Poisson problem and two *linearized* convection-diffusion equations.
Gummel's map reads as follows.

Outer iteration: Loop on k until convergence

- Construct Newton iterates $\{\psi_m^k\}$ for the nonlinear elliptic boundary value problem

$$(9)\quad \begin{cases} -\psi''^k = (\rho_p^{k-1} e^{-\psi^k} - \rho_n^{k-1} e^{\psi^k} + C(x)) = \rho(x, \psi^k(x)), & 0 < x < L \\ \psi^k(0) = \psi_0, \qquad \psi^k(L) = \psi_L \end{cases}$$

such that

$$\lim_{m \to \infty} \psi_m^k = \psi^k$$

Inner iteration:

- for each m solve the linearized problem by the Neumann-Neumann (NN) multidomain method proposed in [1].

- Solve the two linear drift-diffusion problems

$$(10)\quad \begin{cases} -(\mu_n^k(n'^k - n^k \psi'^k))' = -R(\psi^k, n^{k-1}, p^{k-1}), & 0 < x < L \\ n^k(0) = n_0, \qquad n^k(L) = n_L \end{cases}$$

$$(11)\quad \begin{cases} -(\mu_p^k(p'^k + p^k \psi'^k))' = -R(\psi^k, n^{k-1}, p^{k-1}), & 0 < x < L \\ p^k(0) = p_0, \qquad p^k(L) = p_L \end{cases}$$

for n^k and p^k by the NN multidomain method (upon "symmetrizing" the convection-diffusion problems)

The intermediate nonlinear step (9) provides a new electric potential ψ^{k+1} which is plugged into the two convection-diffusion equations to be solved for the carrier concentrations n^{k+1} and p^{k+1} respectively. The procedure is stopped as soon as the variations of electric potential and carrier concentrations between two consecutive iterations (for a suitable norm) fall below a fixed tolerance.
The finite element method is used for the spatial approximation, where piecewise linear and exponentially fitted (*à la* Scharfetter-Gummel (SG) [7]) shape functions are respectively employed for electric potential and carrier densities (see also [2] and [6]).

Use of a Neumann-Neumann domain decomposition method is motivated by the strongly varying nature of the solutions of realistic semiconductor device problems. Indeed, they typically exhibit very sharp interior layers across the p-n junctions where convection dominates and whose position may be easily determined *a priori*, while they behave smoothly in the rest of the device domain. The Neumann-Neumann domain decomposition method allows the solution of self-adjoint boundary-value problems in regions partitioned into subdomains through an iterative procedure among subdomains. At each step the updating is achieved

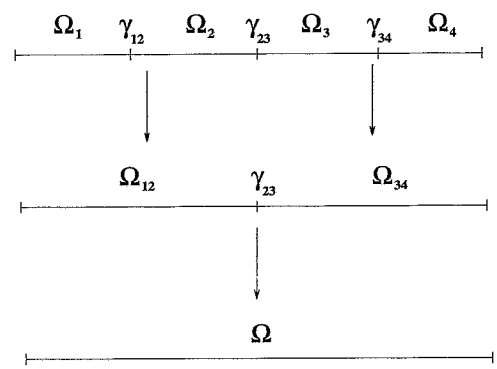

Figure 1: Recursive partitioning algorithm to reduce to single interface problems

by solving independent subproblems with Dirichlet conditions; this phase is followed by a correction yielding subproblems with Neumann conditions at the interfaces among subdomains. The method is described in [1], where an acceleration procedure relying on Conjugate Gradient (CG) iterations for the so called Steklov-Poincare's interface operator is also proposed.

We may interpret this algorithm at the continuous level by saying that, starting from an initial guess u^0, the NN method generates a sequence of approximants $\{u^n\}$ of the exact solution; such functions are continuous over the device domain Ω but, in general, will have discontinuous derivatives at the interfaces. The Neumann step serves to smooth these irregularities by smearing the jumps at each interface of the electric field and of the discrete current densities all over the subdomains.

As for the numerical treatment of current continuity equations, there are two conflicting needs to be satisfied, namely, the self-adjointness of the operators and the computation of exponential terms arising from the change of variables (7)-(8) that make these equations self-adjoint. The successful strategy (*cf.* [5]) consists in modifying the standard Neumann-Neumann method in such a way as to solve a series of differential problems having *just one* interface each, and, consequently, only one degree of freedom. This kind of subproblem may be in fact easily solved in a *single* iteration by the original domain decomposition procedure.

Actually, the starting coupled problem partitioned in N subdomains is *recursively* led to $N/2$ subdomains problems by an algorithm that systematically eliminates the interfaces until *single-interface* problems are reached and eventually solved. This strategy is illustrated in figure 1 in the case of $N = 4$.

4 Numerical results

In this section we discuss some numerical examples relative to the simulation of a one dimensional p-n diode with an abrupt doping profile $C(x)$ and subject to some different values of the biasing potential $V_a = V_{ap} - V_{an}$, where V_{ap}, V_{an} are

respectively the external applied potentials at $x = 0, L$. We assume the device length L = 10μm (junction at $x = \mathrm{L}/2$) and the piecewise constant doping profile

$$(12)\quad C(x) = \begin{cases} -10^{17} cm^{-3} & 0 \le x \le \frac{L}{2} \\ 10^{17} cm^{-3} & \frac{L}{2} < x \le L \end{cases}$$

We show in figure 2 the numerical results relative to the simulation of the p-n diode at the *reverse bias* $V_a = -15$ Volt (i.e., $V_a < 0$). Sharp interior layers across the junction are clearly exhibited by both electric potential and carrier distributions; the former are due to the discontinuity in the doping profile $C(x)$, while the highly dominating transport E $= -\psi'$ around the p-n junction is responsible for the latter. The main parameters of the simulation are sketched in the headings, where IDOM is the number of subdomains, NP is the total number of internal nodes and ITGLOB denotes the number of iterations on k needed to achieve convergence of Gummel's map. Notice the highly nonuniform distribution of the mesh nodes over the device domain; the grid spacing has been taken constant within each subdomain, being quite coarse in the lateral quasi neutral regions and much finer in the depleted zone across the junction, where the maximum variations of the solutions are expected.

We stress that the solution by the NN domain decomposition method of each subproblem has always required a *number of iterations as low as the number of interfaces*. We also remark the effectiveness of the SG finite elements in reproducing the sharp interior layers exhibited by the carrier distributions.

Other examples of simulations of the p-n diode test device under different biasing conditions are reported in [5], with special emphasis on the case of a *high reverse voltage* V_a. The results show the quick convergence of the non linear block iterative procedure, which turns out to be reasonably independent of the applied voltage V_a; further checks on the discrete distributions of electric potential and carrier concentrations have also proved the accuracy of the method measured in the sup-norm.

It must be pointed out that convergence of the Gummel's map quickly worsens as the reverse bias assumes increasing negative values, until it definitevely stops as V_a approaches the breakdown voltage (see, e.g. [9]). The numerical solution of the drift-diffusion system in this physical situation is extensively addressed in [5], where a very effective variant of Gummel's map based on BI-CGSTAB [10] preconditioned iterations is proposed.

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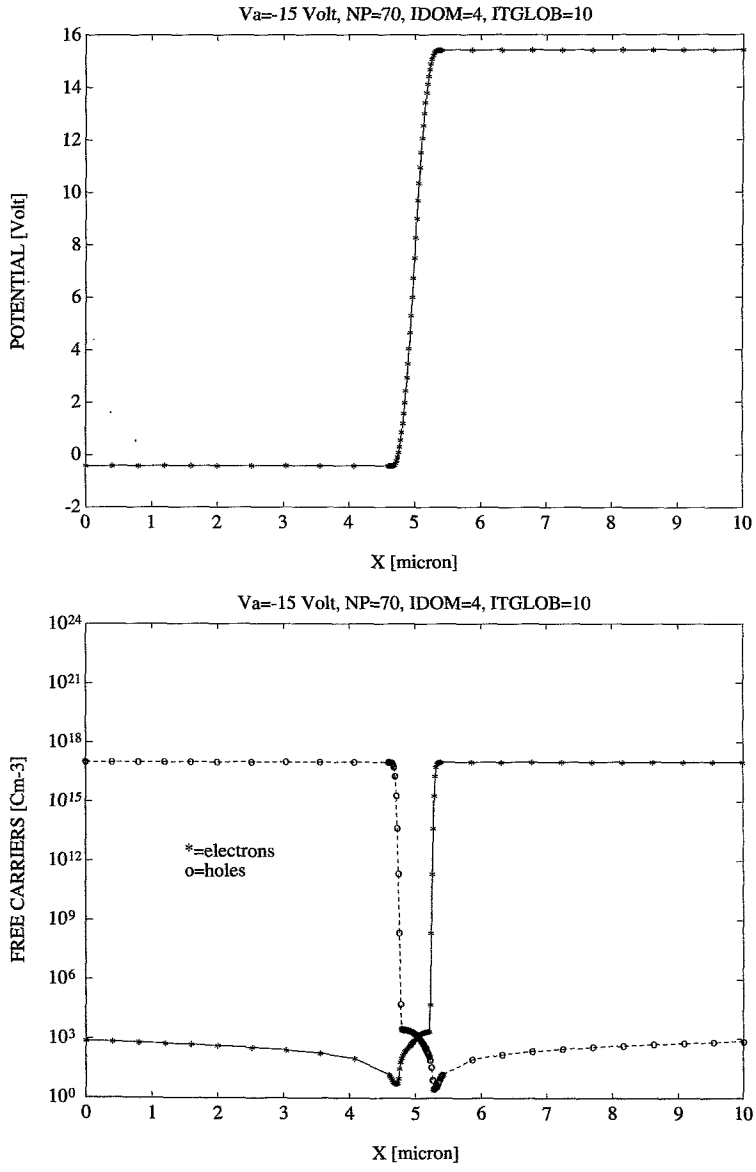

Figure 2: Potential and carrier distributions at $V_a = -15$ Volt

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