SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 5
Edited by S. Selberherr, H. Stippel, E. Strasser – September 1993

Improvement of Initial Solution Projection in Solving General Semiconductor Equations Including Engery Transport

L. L. So, D. Chen[†], Z. Yu[‡], and R. W. Dutton[‡]

Applied Theoretical Physics Division, Los Alamos National Laboratory
Los Alamos, NM 87545, USA
[†]Linear Process Development, National Semiconductor Corporation
2900 Semiconductor Drive, Santa Clara, CA 9502, USA
[‡]Integrated Circuits Laboratory, Stanford University
Stanford, CA 94305, USA

Abstract

An extension of Newton iteration method which provides an effective way to project an initial guess for a subsequent bias conditions – Newton projection Method (NPM) – is described. In particular, we applied the NPM to a system of semiconductor device equations including energy transport. The computational advantages of initial guess projection via NPM are illustrated through examples.

1. Introduction

It is well known that the closeness of the initial guess to the final solution is one of the most critical steps in solving nonlinear equations using the Newton-Raphson iterative method. Although there are several initial guess schemes such as "extrapolation" and "previous" currently adopted in popular semiconductor device simulators, each of these schemes has its limitation. Especially when the problem itself becomes more nonlinear, which is the case when the energy transport equations are added to the conventional drift-diffusion model, finding an effective way to project a "good" initial guess is very crucial.

We have endured a very difficult experience in achieving the convergence for solving the device characteristics once the carrier temperatures are included in addition to the electrostatic potential and carrier concentrations. In particular, when the device is in the operation region where the terminal currents are small, the bias steps have to be limited to about 50 mV for both diodes (e.g., ballistic $n^+ - n - n^+$) and BJTs. The underlying reason is that the carrier temperatures change very rapidly over a short distance, adding severe nonlinearity to the semiconductor problem.

In this work, we describe the extension of Newton Projection Method (NPM) [1] in solving semiconductor equations including energy transport equations[2, 3]. The central idea of the proposed algorithm is to treat biases, which enter into the system

[1]Presently with Applied Theoretical Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545.

[2]Presently with Linear Process Development, National Semiconductor Corp., Santa Clara, CA 95052.

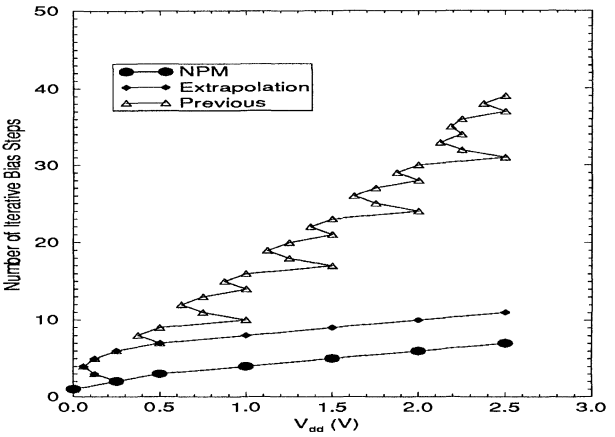

Figure 1: Comparison of the total number of required iterative bias steps of different initial guess schemes for a 1-μm silicon $n^+ - n - n^+$ diode.

is shown in Fig. 1. As expected, the case in which only the previous solution is used has the worst performance. A built-in mechanism which automatically cuts by half the magnitude of the bias step has to be frequently invoked whenever a convergence problem is encountered. Hence each back-tracking (converged or yet-to-be-convergenced) step is being counted into the total number of iterative steps required because of the actual computational cost involved. Although it is possible to use smaller bias steps initially to reduce the cost of back-tracking, it is rather difficult to achieve during a dynamic biasing cycle since it is nearly impossible to have a priori knowledge of what the optimal magnitude for the bias steps should be. While the "extrapolation" method renders some improvement especially in the high bias region, considerably smaller bias steps (about 50 mV) are required near the equilibrium, where the distribution of the carrier temperatures is very nonlinear with respect to the applied voltage. Fig. 2 illustrates the distribution of the majority carrier temperature along the device at small biases.

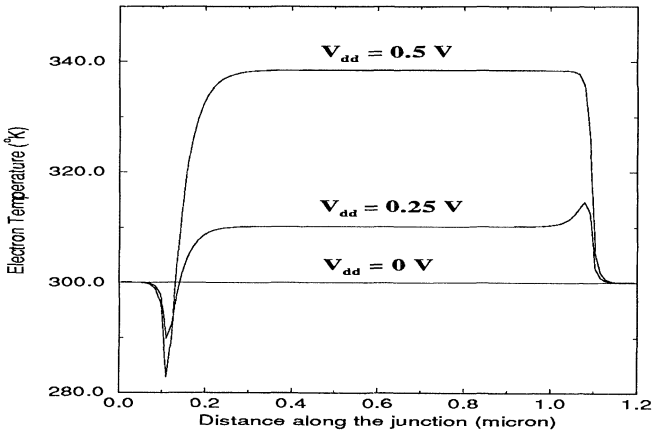

Figure 2: Electron temperature distribution along silicon $n^+ - n - n^+$ diode.

In a bipolar transistor, biases are required to change for both V_{BE} and V_{CE} in order to simulate the I-V characteristics. The number of iterative bias steps required for solution when employing different initial guess schemes as V_{CE} increases for an NPN transistor is shown in Fig. 3. Again, while the convergence behavior of the "extrapolation" method

of semiconductor equations through the boundary conditions, as variable parameters along with the basic equation variables, such as electrostatic potential, carrier concentrations and carrier temperatures. The variation of these quantities with respect to the change of applied bias at the current operation point is readily obtainable through a single Gaussian elimination step, given the Jacobian matrix. Thus by knowing the the functional dependence of the potential, carrier concentrations and temperature distribution on bias, a first order approximation of the solution for the next bias point can be constructed and can be used as an initial guess for the Newton iteration for a subsequent bias.

2. Proposed Algorithm

Consider a semiconductor system consisting of the basic quantities – potential ψ, the carrier concentrations n and p, the carrier temperatures T_n and T_p. The goal for a dc solution is to find a vector $\mathbf{x}$ for each fixed bias condition $\mathbf{V}_o$ for the following equation:

$$\mathbf{f}(\mathbf{x}, \mathbf{V}_o) = 0. \tag{1}$$

Here the vector $\mathbf{f}$ consists of the Poisson equation, carrier continuity equations and energy balance equations at each grid point. The solution vector has the form

$$\mathbf{x} = (\psi_1, n_1, p_1, Tn_1, Tp_1, \cdots, \psi_N, n_N, p_N, Tn_N, Tp_N)^T,$$

with the subscript N representing the number of grid points in the solution region. The bias $\mathbf{V}_o$ enters the equation as a boundary condition and is treated generally as a fixed parameters.

By the use of the Newton Projection Method, the first order approximation to the solution at a subsequent bias can be evaluated using the Taylor expansion of (1)

$$\mathbf{f}(\mathbf{x}_o + \Delta\mathbf{x}, \mathbf{V}_o + \Delta\mathbf{V}) = \mathbf{f}(\mathbf{x}_o, \mathbf{V}_o) + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{(\mathbf{x}_o, \mathbf{V}_o)} \Delta\mathbf{x} + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{V}}\right|_{(\mathbf{x}_o, \mathbf{V}_o)} \Delta\mathbf{V} = 0 \tag{2}$$

where $\mathbf{x}_o$ represents the dc solution. Because of the fact that $\mathbf{f}(\mathbf{x}_o, \mathbf{V}_o) = 0$, the above equation reduces to

$$\left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{(\mathbf{x}_o, \mathbf{V}_o)} \Delta\mathbf{x} = -\left.\frac{\partial \mathbf{f}}{\partial \mathbf{V}}\right|_{(\mathbf{x}_o, \mathbf{V}_o)} \Delta\mathbf{V} \quad . \tag{3}$$

Here the Jacobian matrix $\partial\mathbf{f}/\partial\mathbf{x}|_{(\mathbf{x}_o, \mathbf{V}_o)}$ is already known from the last Newton iteration for the dc solution, and the vector on the right hand side $\partial\mathbf{f}/\partial\mathbf{V}|_{(\mathbf{x}_o, \mathbf{V}_o)}\Delta\mathbf{V}$ which relates the system $\mathbf{f}$ to the boundary condition $\mathbf{V}$ has a relatively simple form. Hence the solution $\Delta\mathbf{x}$ in Eq. (3) is straighforward since only one Guassion elimination step is involved. Since there is no iteration is required, the compution effort is minor.

In the case of a non-negligible magnitude of $\Delta\mathbf{V}$, such as bias step advances, $\mathbf{x} + \Delta\mathbf{x}$ represents a first-order approximation to the solution of system at the new bias of $\mathbf{V}_o + \Delta\mathbf{V}$. Thus it can be used as an initial guess for the final solution at the new bias.

3. Device Examples

We simulated a 1-μm silicon $n^+ - n - n^+$ diode using the ET model, starting from equilibrium condition up to V_{dd}=2.5 V using some fixed bias steps. The number of iterative bias steps required for solution when employing different initial guess schemes

is comparable to NPM at large bias, the NPM is superior near the equilibrium. A consistent bias steps of 0.25 V can be used throughout the simulation region without incurring convergence problem.

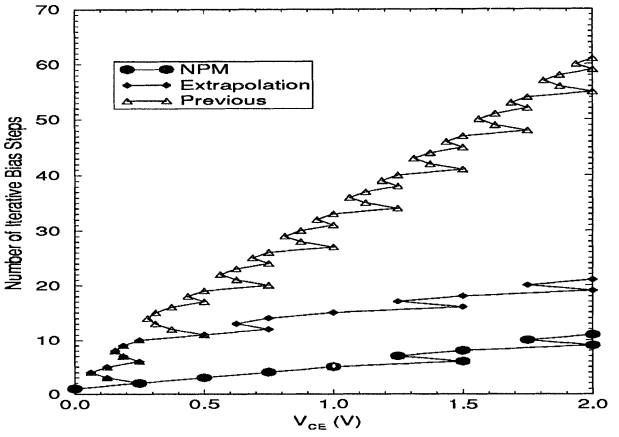

Figure 3: Comparison of the total number of required iterative bias steps of for an NPN bipolar transistor.

4. Conclusions

We have applied the NPM to semiconductor device modeling including energy transport equations. We have shown that the NPM can enhance the rate of convergency during bias advancing over conventional project methods by providing a better initial guess solution, especially when severe nonlinearity are present in the device equations. The improvement in the initial guess permits application of larger bias steps. Additionally, the advantages of the NPM over conventional projection method are two-fold. First, it is based only on the solution at the previous operation point, whereas the conventional extrapolation method needs at least two previous bias points. Hence the method can start even from the equilibrium solution. Second, since the change in bias is not limited to the scalar variable, the prediction can be made when the biases at the different contacts change with different magnitudes.

References

[1] Z. Yu, R. W. Dutton, and M. Vanzi, "An extension to Newton's Method in Device Simulators - On an efficient algorithm to evaluate small-signal parameters and to predict initial guess," *IEEE Trans. Computer-aided Design*, vol. CAD-6, no. 1, pp. 41-45, Jan. 1987

[2] D. Chen, E. C. Kan, U. Ravaioli, C. Shu and R. W. Dutton, "An improved energy transport model including non-parabolic and non-Maxwellian distribution effects," *IEEE Elec. Dev. Lett.*, vol. 13, no. 1, pp. 26-28, Jan. 1992.

[3] D. Chen, E. Sangiorgi, M. R. Pinto, E. C. Kan, U. Ravaioli and R. Dutton, "Analysis of spurious velocity overshoot in hydrodynamic simulations of ballistic diodes," *Proceeding of NUPAD V (Numerical Process and Device Modeling Workshop)*, Seattle, May 31 - June 1, 1992.