A New, Easy-to-Code, Robust and Stable Approach to 2-D Hydrodynamic Submicron Device Modeling

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I. Introduction

We present a new technique for solving the Hydrodynamic(HD) equations in submicron device simulations. This method is extremely stable, quickly converges even with poor initial guesses, and agrees with Monte Carlo(MC) calculations. In addition, this new method is easy to code for 2-D device simulation. We have applied the new method to simulate 2-D MOSFETs as well as SOI devices.

To our knowledge, no agreed-upon HD model has emerged as the basis for a standard device simulator. The lack of an industry-standard CAD tool can be attributed to the difficulties in obtaining an accurate, numerically stable, and rapidly convergent solution to the HD equations. We have developed a new robust algorithm for HD device simulation that overcomes existing difficulties. We formulate the HD equations into self-adjoint forms with a new set of Slotboom-like state variables. The discretizations result in a diagonally dominant coefficient matrix for each HD equation. Consequently, the convergence of each equation is guaranteed for any initial guess when iterative solution methods are employed. Our discretization technique resolves the rapid spatial variations which may occur in carrier densities and carrier temperatures. As a result, stability of the HD solution is improved. Furthermore, a fixed-point iterative method is employed to determine the solution of each discretized HD equation. A direct solution of a matrix equation is therefore avoided. In addition, the method requires little memory, and is well-suited for parallel computations.

II. The HD Model

The HD equations are obtained from a standard HD formulation [1].

$$\nabla^2 \phi = \frac{q}{\epsilon_s}(n - p - D) \tag{1}$$

$$\frac{1}{q} \nabla \cdot \vec{J}_n = R \tag{2}$$

$$\nabla \cdot \vec{S}_n = \vec{J}_n \cdot \vec{E} - n\frac{\omega_n - \omega_o}{\tau_{n\omega}(T_n)} \tag{3}$$

$$\vec{J}_n = -q\mu_n n \nabla \phi + qD_n \nabla n + \mu_n k_B n \nabla T_n \tag{4}$$

$$\vec{S}_n = \frac{\vec{J}_n}{-q}\omega_n + \frac{\vec{J}_n}{-q}k_B T_n + \vec{Q}_n \tag{5}$$

$$\omega_n = \frac{2}{3} k_B T_n + \frac{1}{2} m_n^* v_{dn}^2 \tag{6}$$

$$\vec{Q}_n = -\kappa_{cn} \nabla T_n, \qquad \kappa_{cn} = 2T_n (k_B/q)^2 (n q \mu_n) \tag{7}$$

Here, ϕ is the electric potential; n and p are the electron and hole densities respectively; D is the net doping concentration; $\vec{J}_n$ is the electron current density; R denotes the recombination process; ω_n is the average electron energy and $\vec{S}_n$ is the electron energy flux; $\vec{E}$ is the electric field; $\tau_{n\omega}$ is the energy relaxation time for electrons; ω_o is the average carrier energy in thermal equilibrium; μ_n is the electron-temperature-dependent mobility; D_n is electron temperature-dependent diffusivity; T_n is the electron temperature; m_n^* is electron effective mass; v_{dn} is the electron mean velocity; $\vec{Q}$ is the heat flux. (We note that, in an effort to be concise, only the HD equations for electrons were shown. However, our calculations include the self-consistent solution of the hole and electron HD equations.)

The typical approach at this point is to solve the above system of equations by using n, T_n as the unknown state variables. However, the current-continuity and the energy-balance equations under this approach may give rise to numerical difficulties such as stability problems and spurious spikes in average electron velocity. To overcome these numerical problems, we take another approach by first defining a new set of Slotboom-like state variables. Then, we transform the HD equations into self-adjoint forms with these new variables. A new Scharfetter-Gummel-like discretization scheme is then employed to resolve the rapid variations in n and T_n. The resulting matrix equations are diagonally dominant and exhibit excellent numerical properties.

III. The New Method for Solving HD Equations

A. Slotboom-Like Variables for the HD Model

We define a new set of Slotboom-like state variables u and g_n for electron density and electron temperature:

$$n = n_i \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q(\phi - \psi_n)}{k_B T_L}\right) = n_i u \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}\right) \tag{8}$$

$$u = \exp\left(-\frac{q\psi_n}{k_B T_L}\right) \tag{9}$$

$$T_n = g_n \exp(\psi_n / a_T), \quad a_T = \frac{\kappa_{cn}}{\frac{5}{2}\mu_n n k_B} = \frac{4}{5}\frac{k_B T_L}{q} = 0.0207V \tag{10}$$

where ψ_n is the electron quasi-Fermi potential and T_L is the lattice temperature.

B. The Self-Adjoint form of the HD model

Substituting eqns. (8)(9) into (4), and eqn. (10) into (5) respectively, the electron current density and electron energy flux in terms of the Slotboom-like variables u and g_n are as follows:

$$\vec{J_n} = D_n n_i \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}\right) \bigtriangledown u, \tag{11}$$

$$\vec{S_n} = -\kappa_{cn} \exp(\psi_n/a_T) \bigtriangledown g_n + \frac{\vec{J_n}}{-q}(\frac{1}{2} m_n^* v_{dn}^2). \tag{12}$$

Eqn. (11) can be further simplified to $\vec{J_n} = -q\mu_n n \bigtriangledown \psi_n$. The steady state HD model can now be described by a system of self-adjoint equations. This system can be obtained by appropriately substituting eqns. (11)-(12) into eqns. (1)-(3).

$$\bigtriangledown^2 \phi = \frac{qn_i}{\epsilon_s}\left(u \exp(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}) - v \exp(-\frac{T_p - T_L}{T_L} - \frac{q\phi}{k_B T_L})\right) - \frac{qD}{\epsilon_s} \tag{13}$$

$$\bigtriangledown \cdot \left(D_n n_i \exp(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}) \bigtriangledown u\right) = R(\phi, u, v) \tag{14}$$

$$\bigtriangledown \cdot (\kappa_{cn} \exp(\psi_n/a_T) \bigtriangledown g_n) = n\frac{\frac{3}{2} k_B g_n \exp(\psi_n/a_T) + \frac{1}{2} m_n^* v_{dn}^2 - \omega_o}{\tau_{n\omega}} - \vec{J_n} \cdot \vec{E} - \bigtriangledown \cdot \left(\frac{\vec{J_n}}{q} \frac{1}{2} m_n^* v_{dn}^2\right) \tag{15}$$

It is clear from the above expressions that the Poisson, the current-continuity and the energy-balance equations are each self-adjoint differential equations with respect to the variables ϕ, u and g_n. It is also interesting to note that when T_n is equal to T_L, the above new expressions for the Poisson and current continuity equations reduce to the DD model[2].

C. Discretization Scheme and Iterative Method for HD Equations

A Scharfetter-Gummel-like method is employed to discretize the current-continuity equations and the energy-balance equations. The discretizations result in a diagonally dominant coefficient matrix for each HD equation. A fixed-point method is applied to solve the system of discretized HD equations. Due to the property of diagonal dominance, the convergence for the solution of each HD equation is guaranteed [2,3].

IV. Numerical Results

To test convergence of the technique, we generated initial guesses using a random function. With random initial guesses, the same results were obtained as when good initial guesses were used. To examine stability, we simulated MOSFET's on a rather coarse grid of less than 400 mesh-points and smooth results were obtained. Additionally, we found that, in general, our HD simulations required only about 75% more CPU time than drift-diffusion model simulations. Fig. 1 shows the simulation results for a submicron MOSFET with $0.5\mu m$ channel length. In Fig. 2, we show the results of a computation performed for a $1\mu m$-channel SOI device. Finally, to test the accuracy of the new HD model, we compared our simulations to MC calculations for a square shape

field. Fig. 3 shows good agreement between MC simulations and our HD calculations. Also interesting in Fig. 3 is that the spurious second overshoot spike, which usually appears in HD simulations, is absent from our calculations.

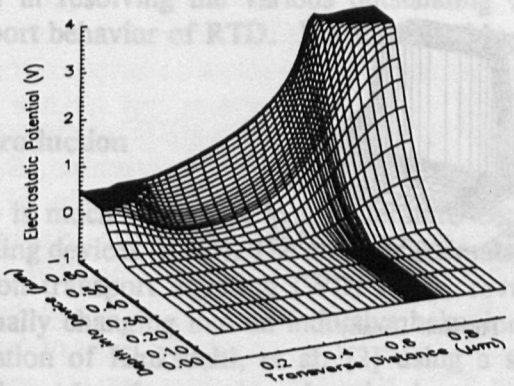
References

[1] K. Blotekjaer, *IEEE Trans. Electron Dev.*, vol. ED-17, pp.38, 1970

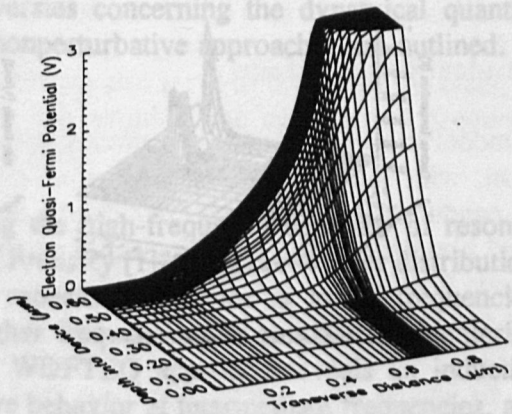
[2] C. Korman and I. D. Mayergoyz, *Journal of Appl. Phys.*, 68 (3), pp. 1324-1334, 1990

[3] Q. Lin, N. Goldsman and G.-C. Tai, *Solid-State Electron*, vol. 36, no. 3, pp. 411-419, 1993.

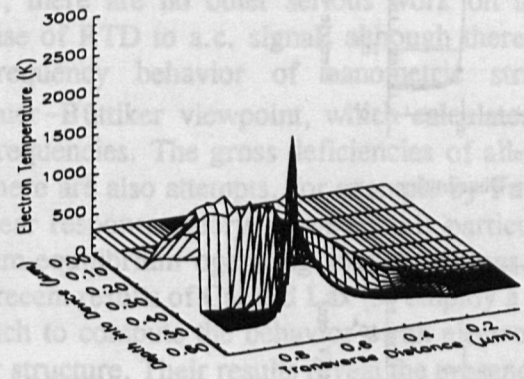
Figure 1. 2-D Submicron MOSFET Simulation Results
(Vgs = $3V$, Vds = $3V$, Channel Length = $0.5\mu m$)



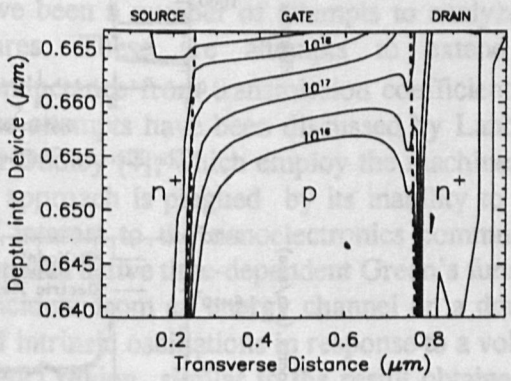
The Electrostatic Potential



The Electron Quasi-Fermi Potential

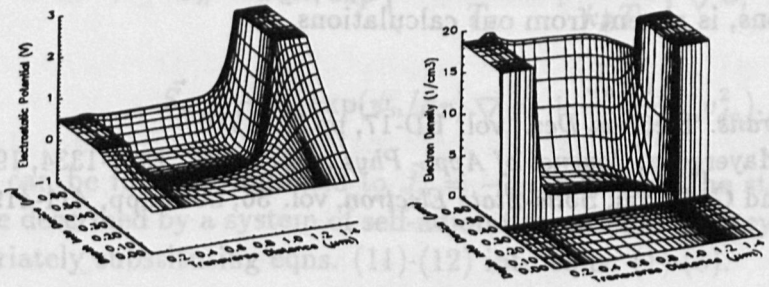


The Electron Temperature

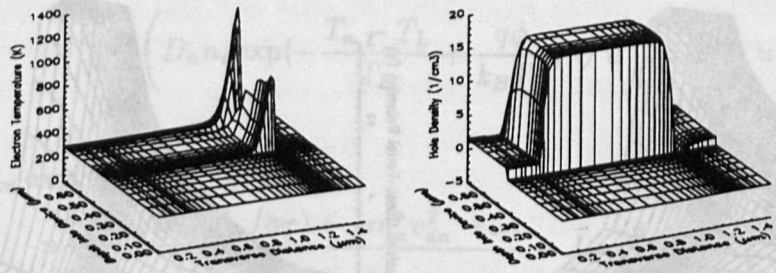


The Electron Density

Figure 2. 2-D Partially Depleted SOI MOSFET Simulation Results
(Vgs = 2V, Vds = 2V, Channel Length = $1\mu m$)

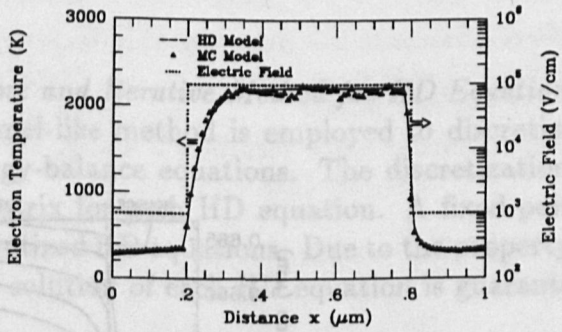


The Electrostatic Potential The Electron Density

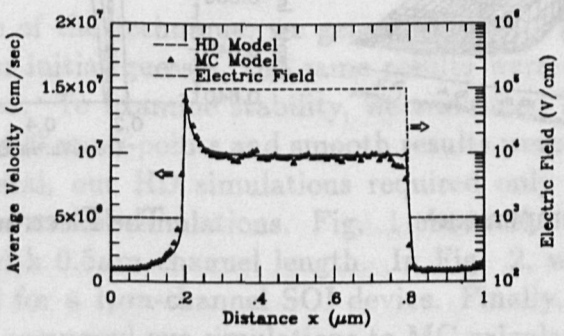


The Electron Temperature The Hole Density

Figure 3. Comparision between HD and MC Calculations



The Electron Temperature Distribution



The Electron Average Velocity Distribution