Three-Dimensional Hydrodynamic Simulation of Submicron MOSFET's

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Abstract

This paper presents a method for solving the 3-D hydrodynamic (HD) model in submicron semiconductor devices. The main features of this method are the fairly low memory and CPU time requirements, and excellent convergent property. Simulation results of a 3-D submicron MOSFET are provided.

I. Introduction

As device dimensions continue to shrink, 3-D-related phenomena, including the MOS bird's beak and narrow channels effects, can significantly impact device characteristics. As a result, demand for 3-D simulations has appeared [1,2]. As far as we know, very few robust 3-D device simulators exist, and we know of none which are based on the hydrodynamic model. In general, the HD model is difficult to solve because it is a highly nonlinear, singularly perturbed, highly coupled system of partial differential equations. While these difficulties are readily evident in 2-D, they are compounded when 3-D simulations are attempted. In addition to the standard obstacles of traditional 2-D simulations, the increased difficulties for 3-D simulation can be summarized as follows: (1) Memory: 3-D simulation of electrons and holes requires the solution of between 10⁵ and 10⁶ simultaneous discrete equations. Use of the standard Newton's method requires storing extremely large matrices to accomodate this large number of discrete equations. (2) Algorithm: Solving such large matrices is very difficult and readily leads to round-off errors and instabilities. (3) Boundary conditions in 3-D are more complicated than their 2-D counterparts, which leads to changes in the matrix structure and more difficulties when nonplanar surfaces are encountered. (4) Convergence and stability: More complicated coupling relations between mesh points and between equations significantly increase the nonlinearities already associated with the HD model.

We have overcome numerical problems associated with 3-D HD modeling, and developed an efficient 3-D HD simulator for predicting deep-submicron MOSFET performance. Instead of using solution techniques, such as Newton's method or the conjugate gradient approach, we adapt our solution approach specifically for 3-D HD device simulation. This required extending our highly stable and routinely convergent method for 2-D HD modeling to 3-D[3,4],

To tailor our approach specifically for the 3-D problem, we use a fixed point iterative approach which totally avoids solving large matrices. By defining new Slotboom-like variables for the HD model, we transform the original HD equations to self-adjoint form which guarantees that each discretized HD equation will correspond to a diagonally dominant matrix. A Scharfetter-Gummel-like (S-G) discretization is then performed on the self-adjoint forms of the current-continuity and energy balance equations. The S-G-like schemes resolve rapid variations of unknown variables, not only due to the mesh refinement, but due to the special design of the finite difference schemes as well, thereby helping to reduce the number of mesh-points, equations, and time to convergence. The coupled system is solved using SOR-type methods where the equation for each mesh point is updated explicitly. The explicit method obviates the need

to solve large matrices, and, due to the diagonal dominance, each HD equation is guaranteed to converge[5,6]. The explicit method is independent of matrix structure so implementing additional 3-D related boundary conditions do not noticeably affect the solution. Furthermore, memory requirements of the fixed-point iteration method are fairly low, thereby facilitating solution in 3-D. Finally, the explicit method is intrinsically parallel.

II. Solution of 3-D HD Equations

The Self-Adjoint form of the HD model

To solve the HD model in 3-D, we begin with the standard HD equations[7]. By using the Slotboom-like variables variables u, v, g_n, g_p for the standard HD variables n, p, T_n, T_p , the electron current density and electron energy flux can be expressed in the compact form:

$$\vec{J_n} = D_n n_i \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}\right) \bigtriangledown u, \tag{1}$$

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

$$u = \exp\left(-\frac{q\psi_n}{k_B T_L}\right), \quad T_n = g_n \exp(\psi_n/a_T), \quad a_T = \frac{\kappa_{cn}}{\frac{5}{2}\mu_n n k_B} = \frac{4}{5} \frac{k_B T_L}{q} = 0.0207V \quad (3)$$

By substituting above expressions into the original HD equations, one can transform the HD model into self-adjoint form:

$$\nabla^2 \phi = \frac{qn_i}{\epsilon_s} \left(u \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}\right) - v \exp\left(-\frac{T_p - T_L}{T_L} - \frac{q\phi}{k_B T_L}\right) \right) - \frac{qD}{\epsilon_s}$$
(4)

$$\nabla \cdot \left(D_n n_i \exp\left(-\frac{T_n - T_L}{T_L} + \frac{q\phi}{k_B T_L}\right) \bigtriangledown u \right) = R(\phi, u, v) \tag{5}$$

$$\nabla \cdot (\kappa_{cn} \exp(\psi_n/a_T) \bigtriangledown g_n) = n \frac{\frac{3}{2} k_B g_n \exp(\psi_n/a_T) + \frac{1}{2} m_n^* v_{dn}^2 - \omega_o}{\tau_{n\omega}} - \vec{J_n} \cdot \vec{E} - \nabla \cdot \left(\frac{\vec{J_n}}{q} \frac{1}{2} m_n^* v_{dn}^2\right)$$
(6)

It is clear from the above expressions that the Poisson, the current-continuity, and the energybalance equations are each self-adjoint differential equations with respect to the variables ϕ , uand g_n .

Iterative Method for HD Equations

We use an S-G-type method to discretize the current-continuity and energy-balance equations. This S-G approach helps to analytically resolve the rapid variations in n and T_n , thereby reducing the number of mesh-points which can become quite large for 3-D applications. With the S-G-like discretization, we assume that S_n and J_n are constant between mesh-points. Integration of the above self-adjoint forms between the mesh-points is then readily performed. The overall variation of S_n and J_n is then accounted for discretely on the mesh-points. This discretization yields the following 3-D general expression for the current-continuity and energybalance equations:

$$c_{i+1,j,k}H_{i+1,j,k} + c_{i-1,j,k}H_{i-1,j,k} + c_{i,j+1,k}H_{i,j+1,k} + c_{i,j-1,k}H_{i,j-1,k} + c_{i,j,k+1}H_{i,j,k+1} + c_{i,j,k-1}H_{i,j,k-1} - (c_{i+1,j,k} + c_{i-1,j,k} + c_{i,j+1,k} + c_{i,j-1,k} + c_{i,j,k+1} + c_{i,j,k-1} + L_{i,j,k})H_{i,j,k} = -\gamma_{i,j,k}$$

$$(7)$$

In the above equation $H_{i,j,k}$ represents the discrete form of the Slotboom variable either u or g_n . The c's are the discretization coefficients corresponding to each HD equation. $L_{i,j,k}$ represents the diagonal term arising from the RHS of the self-adjoint equations, while $\gamma_{i,j,k}$ represents the 'constant' term on the RHS of eqns.(5) and (6). It is interesting to note that the discretization of the self-adjoint forms yields coefficient matrices which are diagonally dominant. This can be observed since all the coefficients $c_{i,j,k}$, as well as $L_{i,j,k}$, have the following property:

$$c_{i+1,j,k} \ge 0, \quad c_{i-1,j,k} \ge 0, \quad c_{i,j+1,k} \ge 0, \quad c_{i,j-1,k} \ge 0, \quad c_{i,j,k+1} \ge 0, \quad c_{i,j,k-1} \ge 0, \quad L_{i,j,k} \ge 0.$$
(8)

Eqn.(7) represents a system of $N = (N_i \times N_j \times N_k)$, where N_i, N_j, N_k represent the number of meshpoints in each dimension, respectively. Ordinarily, such a system would be solved implicitly using a Newton-type approach. However, such an approach would yield extremely large matrix equations which have extensive memory requirements and are susceptable to round-off error.

Our approach, which has been specially tailored for hydrodynamic 3-D applications, allows for eqn.(7) to be solved explicitly, thereby avoiding large matrices entirely. We solve eqn.(7) for $H_{i,j,k}$, a fixed-point method, such as Jacobi iteration technique, is then applied to update the HD-Slotboom variable at each mesh-point using the following equation:

$$H_{i,j,k}^{(n+1)} = \frac{A_{i,j,k}^{(n)} + \gamma_{i,j,k}}{B_{i,j,k} + L_{i,j,k}}$$
(9)

where $A_{i,j,k}^{(n)}$ represents the sum of the off-diagonal 'cH' terms in eqn.(7), and $B_{i,j,k}$ represents the sum of the 'c' coefficients of the diagonal term $H_{i,j,k}$.

This iteration scheme minimizes memory allocation, requiring only a few vectors of length N. Furthermore, due to the property of diagonal dominance, the convergence for the solution of each HD equation is guaranteed [4,5], while the convergence of the overall system is obtained with a modified Gummel method. Finally, by observing the decoupled algorithm of eqn.(9), it is clear that the method is readily parallelized.

III. Numerical Results

To examine the new method, we simulated a semi-recessed, 3-D submicron MOSFET, as shown in Fig. 1. The MOSFET has $0.5\mu m$ of channel length and $0.5\mu m$ of channel width. The electron temperature distribution at $V_{ds} = 1.0V$ and $V_{gs} = 3.5V$ is shown in Fig.2. Narrow channel effects can be observed.

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*This work was supported by the Semiconductor Research Corporation.



Fig.1. Semi-recessed MOSFET device with $0.5 \mu m$ effective channel length and $0.5 \mu m$ channel width.



Fig.2. Electron temperature for the device with $V_{drain} = 1.0V$ and $V_{gate} = 3.5V$. (We have enlarged the channel region to show the 3-D effect).