A HYBRID SOLUTION OF THE SEMICONDUCTOR
DEVICE EQUATIONS

by

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Technical Report #649

September 1990
Abstract

The operation of semiconductor devices is often governed by thin transition layers, either near the boundary, or at internal junctions. These regions of large gradients pose tough requirements for the discretization scheme, which is used for the numerical solution of the governing PDE's. These layers are conventionally resolved by extreme local mesh refinement. It has been pointed out that P-N junctions can be effectively discretized by the Scharfetter-Gummel scheme. This method exploits the smoothness of currents through junctions. There has been no similarly successful way to resolve thin channels. We have developed an asymptotic solution of the channel region of MOSFET devices. The aspect ratio of the channel is taken as a small parameter. The layer approximation is imbedded in a hybrid scheme, which computes a correction to the analytic approximation by control-volume discretization. The hybrid method can reach any required accuracy, but overcomes the necessity of highly refined grid in the channel. MOSFET simulations which normally require vast grids were accurately performed by the hybrid method at a drastically reduced cost.
Introduction

State of the art semiconductor simulators are based on finite difference techniques, or on certain combinations of finite elements and finite differences. The extreme gradients which exist in the semiconductor device variables have motivated several attempts to exploit the results of perturbation analysis in order to improve the numerical scheme. The analytic approximations of diodes, which was developed by Markowich, Selberherr, et. al. [6] influenced some aspects of the Bambi simulator. Asymptotic analyses of MOSFET were presented by Brews [1] and by Ward [9]. These solutions are only valid for long channels, and their accuracy is limited.

Our feeling is that a stronger interaction between analytic and numerical methods can lead to more powerful computational methods. The critical components of semiconductor devices are characterized by layers of steep gradients. These are routinely resolved by extreme mesh refinement. On the other hand there is an abundance of engineering literature which analyses transition regions such as junctions and channels, and provide analytic quantitative approximations. It turns out that these layers are often nearly locally one-dimensional, and their leading behavior can be analyzed by perturbation techniques.

Hybrid methods, such as Asymptotic Finite Elements (AFE) [5] [8] provide a framework for a happy marriage between these two types of techniques. A successful implementation of AFE extracts the non-smooth solution components by perturbation methods, and lets the numerical algorithm resolve the correction which is smooth.

As a nontrivial test case we study an N-channel MOSFET configuration (Figure 1 on page 2). This device is quite simple, yet it is representative of many other realistic devices. Under conditions of strong inversion there appears a very thin and steep layer of electrons under the gate. This layer is the controlled channel through which the current flows from source to drain. The following observations will govern our approach:

• The inversion layer is very hard to resolve by difference methods.

• The hole concentration is known to be negligible at a depletion layer. The location of this layer is known and is insensitive to operation parameters.

• The electric potential and the field at the depletion layer are quite well shielded from the gate potential. This isolation is provided by the inversion layer.
Although electron concentration at the channel is very high and sensitive to bias variations, its integral, namely, the charge per unit channel length, varies almost linearly as a function of the gate bias.

It is the total charge which determines the leading order of the channel conductivity, rather than point-wise concentration.

Our aim is hence to try avoiding carrier concentration calculations in the channel, and to use the smooth exterior functions mentioned above for the construction of an external solution.

It should be stressed that unlike most existing asymptotic analyses of the semiconductor equations, the hybrid scheme allows us to reach a solution which is at least as accurate as the existing difference methods. This goal is achieved either by taking more terms of the asymptotic series, or by a numerical solution of the residual error.

Figure 1. A schematic MOSFET device

The general solution scheme is presented in Figure 2 on page 3. A hybrid approximation $u_0$ is computed first, based on an interaction between an inner channel solution and an outer finite volume solution in the rest of the device. This interaction can take the form of inner-outer iterations, or of a Newton linearization procedure. Once this first approximation is complete, we turn to a fully numeric computation of $u_n = u - u_0$. This component can be
effectively discretized on a relatively coarse grid, since $u_\epsilon$ contains the essence of the boundary layer.

Figure 2. The general structure of the hybrid solution.
An Asymptotic solution of a MOSFET

Consider the device in Figure 1 on page 2. Under the influence of an electrostatic field applied at the gate contact, a current flows from source to drain through a thin layer which is located under the insulator interface. This layer of mobile electrons, which forms inside the P-doped region is called an inversion layer. Adjacent to it there is a depletion layer, namely, a region with no mobile carriers. An analysis in [1] reveals that the depletion layer width $W$ is proportional to $\sqrt{\ln C}/C$ where $C$ is channel doping. A horizontal line will be drawn in the middle of this layer. We wish to compute an asymptotic approximation in the rectangular channel region above this line, and an outer solution in the rest of the device. This definition of the 2 domains is designed to insure that the analytic approximation is confined to the depletion layer. A typical geometry is presented in Figure 3.

The small parameter in the channel region is its squared aspect ratio $\delta = (W/(2L))^2$, where $L$ is the channel length. This choice of the squared aspect ratio may seem rather arbitrary but it simplifies the expansions which are used below.

Figure 3. A schematic channel geometry.

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The drift-diffusion equations, expressed in Slotbohm variables and scaled by Qmari's normalization [7] are:

\[ e\Delta \psi - (e^{\psi}\eta - e^{-\psi}p - C) = 0 \]
\[ \nabla (\mu e^{\psi} \nabla \eta) = R \]
\[ \nabla (\mu e^{\psi} \nabla p) = R \]  

(1)

These equations will be solved by an asymptotic expansion in the rectangle ACFH. This channel solution has to match the external numerical solution. The boundary conditions for the channel region are:

\[ \psi, \eta, p \quad \text{prescribed along BC, CF, FG.} \]
\[ \psi = \psi_{\text{gate}} \quad \text{on AH.} \]
\[ \frac{\partial \psi}{\partial x} = 0 \quad \text{on AB, HG.} \]
\[ \frac{\partial \eta}{\partial y} = \frac{\partial p}{\partial y} = 0 \quad \text{on BG.} \]  

(2)

The combination of Neuman and Dirichlet boundary conditions are discussed in the next section, and sketched in Figure 4 on page 8.

A standard procedure for such problems ([2]) is to introduce stretched coordinates. Consider the following set of scaled independent variables:

\[ \tilde{x} = \frac{x}{L} \]
\[ \tilde{y} = \frac{y}{D} \quad \text{where} \quad D = \frac{W}{2} = \frac{1}{2} \sqrt{\lg C_{\text{max}}/C_{\text{max}}} \]
\[ \tilde{C} = D^2 C \quad \text{where} \quad e^{\psi_i} = D^{-2} \]

(3)

The coordinates \( \tilde{x}, \tilde{y} \) now vary in \([0, 1]\), \( \tilde{C} = O(1) \) and \( e^{\psi_i} \approx 1 \) at the edge of the inversion layer. The equations (1) are transformed by this scaling into:

\[ \frac{1}{L^2 D^2} \left( \tilde{\psi}_{xx} + \tilde{\psi}_{yy} \right) = \frac{\eta e^{\psi}}{D^2} - D^2 e^{-\psi} - \frac{\tilde{C}}{D^2} \]
\[ \frac{1}{L^2 D^2} (e^{\psi} \eta_x)_x + \frac{1}{D^4} (e^{\psi} \eta_y)_y = R \]
\[ \frac{1}{L^2} (e^{-\psi} p_x)_x + (e^{-\psi} p_y)_y = R \]  

(4)

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Here we assumed, for simplicity, $\mu = 1$. These equations yield:

$$
\varepsilon (\partial \tilde{\psi}_{xx} + \tilde{\psi}_{yy}) = \eta_0 e^{-\tilde{\psi}} - D^4 p_0 e^{-\tilde{\psi}} - \tilde{C} \\
\delta (e^{\psi} \eta_{\psi}^{xy}) + (e^{\psi} \eta_{\psi})_{xy} = D^4 R \\
\delta (e^{-\psi} p_{\psi}^{xy}) + (e^{-\psi} p_{\psi})_{xy} = R
$$

(5)

Series solutions of the forms:

$$
\tilde{\psi} = \sum_{i=0}^{\infty} \delta^{i} \tilde{\psi}_i, \quad \eta = \sum_{i=0}^{\infty} \delta^{i} \eta_i, \quad \rho = \sum_{i=0}^{\infty} \delta^{i} \rho_i, \quad R = \sum_{i=0}^{\infty} \delta^{i} R_i
$$

(6)

will be sought for. It is not hard to verify that only even terms of the expansions (6) will be present. Collecting leading order terms we obtain:

$$
e^{\psi_{xx}} - \eta_0 e^{\psi_{xx}} = \tilde{C} - D^4 p_0 e^{-\tilde{\psi}} \\
(e^{\psi_0})_{xy} = D^4 R_0 \\
(e^{-\psi_0} p_{\psi_0})_{xy} = R_0
$$

(7)

Considering that $R = O(1)$ and $\delta \approx 10^{-3}$ we can neglect the $D^4$ terms, at least in the first order equations. The first of these equations is a 1D capacitor equation. It will presently be shown that it is unnecessary to fully solve this equation in order to find the leading order current behavior.

The solution of the second equation in (7), considering the Neumann conditions on BG is $\eta_0(\psi_0)$, namely:

$$
\eta_0 = \eta_0(\psi_0)
$$

(8)

In order to recover the actual $\eta_0(x)$ solution we need the second order equations. Collecting coefficients of $\delta$ we obtain:

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The second equation in (9) equations can be integrated with respect to $y$ to yield:

$$\psi_{yy} - \eta_0 \psi + \psi_1 = - \psi_{xx} - \frac{D^2}{\delta} (\rho_0 + \delta \eta_1) \psi_x - \psi_t$$

(9)

Observe that these equations, which are of order 2 in $\delta$ are ODE's in $y$ while their $x$ dependence is parametric. This typical property will prevail in higher order equations.

The second equation in (9) equations can be integrated with respect to $y$ to yield:

$$\int_0^A \left[ e^\psi \eta_0 \right]_x - \left[ e^\psi \eta_1 \right]_x + \int_0^A \frac{D^2}{\delta} (\rho_0 + \delta \eta_1) dy$$

(10)

Here $A$ is some large constant. The bracketed term vanishes at $y = 0$ due to the Neumann condition on BG. It does not vanish at $y = A$, but its coefficient $e^{\psi_0(A)}$ is negligible in comparison to the integral coefficient of the first term. The integration interval can be confined to the layer since the outside contribution is very small. We consequently have:

$$\int_0^1 \left[ e^\psi \eta_0 \right]_x = \int_0^1 \frac{D^2}{\delta} (\rho_0 + \delta \eta_1) dy$$

(11)

Equation (11) is a 1D electron continuity equation with a 'mobility' coefficient which is proportional to the integral of $\psi_x$ across the channel. This is the channel charge per unit length, divided by $\eta$. Let's denote this coefficient as

$$M = M(\eta_0, \eta_1, \psi_{gate} - \psi(x, t))$$

(12)

This integral is a well behaved function, which can easily be interpolated from tabulated values. (11) is now a nonlinear 1D transport equation which can be solved for $\eta_0$ without a detailed knowledge of $\psi_x$. 

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An outer solution

In order to solve the field equation outside the channel we need boundary conditions on the lines BC, CF, FG, (Figure 1 on page 2) in addition to the usual boundary conditions along the device circumference. A global solution of diffusion type equations on decomposed domains can be achieved either by domain overlap, or by Neuman - Dirichlet conditions [3]. The latter option has been chosen for our method. It can be observed in Figure 4 on page 8 that along each of the interface lines both $\psi$ and $\eta$ satisfy Neuman - Dirichlet conditions. As a consequence of the shielding provided by the inversion layer, the normal derivative of $\psi$ along the line CF is almost constant with respect to $\eta$. This mild function is interpolated from a table of 'canned' capacitor solutions. The inner - outer iterations converged fast for the numerical tests which we performed.

The correction to the first order hybrid solution can be achieved either via the second order perturbation equations (9), or numerically, using an AFE procedure. This technique is described in the following section.

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Figure 4. Boundary conditions for inner and outer solutions

8 A Hybrid Solution of the Semiconductor Device Equations
AFE

Israeli and Ungarish [8] suggested a 'booster' method which exploits analytic approximations at the non-smooth domain components, in order to achieve an accurate numerical solution for the problem, without excessive mesh refinement.

The extension of this method to FEM discretization is called Asymptotic Finite Elements (AFE) [4].

Given a linear differential equation:

\[ Lu = f \]  \hspace{1cm} (13)

in a domain \( \Omega \) and boundary conditions

\[ u + \partial u / \partial n = g \]  \hspace{1cm} (14)

which are specified on \( \partial \Omega \), assume that there is an analytic approximation \( u_A \). If the error \( u_n = u - u_A \) is small or smooth, then it can be resolved on a coarse mesh. The method thus solves

\[ Lu_n = f_n = f - Lu_A \]  \hspace{1cm} (15)

The error of the hybrid method is bounded by

\[ \| e_{AFE} \| \leq k \| e_n \| \| e_A \| \] \hspace{1cm} (16)

where \( e_n \) is the error of the numerical solution, and \( e_A \) is the error of the analytic approximation. \( k \) was found to be \( O(1) \). This estimate shows that the hybrid technique combines the merits of the 2 methods.
The semiconductor AFE equations

Poisson's equation and its first order channel approximation are:

\[
\varepsilon \Delta \tilde{\psi} - (\varepsilon \tilde{\psi} - \rho - \psi - C) = 0
\]
\[
\tilde{\psi}_{yy} - \tilde{\psi} - C = 0
\]  

(17)

Subtraction of these equations, and deletion of the hole term give:

\[
\varepsilon \Delta (\tilde{\psi} - \tilde{\psi}_0) - \varepsilon \tilde{\psi} - \tilde{\psi} = - \tilde{\psi} \tilde{\psi}_{ox} - \varepsilon \tilde{\psi}_{ox}
\]

(18)

This 'correction' equation has the same structure as the original equation. This fact is emphasized by the substitution:

\[
\tilde{\psi} = \tilde{\psi} - \tilde{\psi}_0
\]
\[
\tilde{\eta} = \varepsilon \tilde{\psi}_0
\]
\[
\tilde{C} = \varepsilon \tilde{\psi}_{ox} + \varepsilon \tilde{\psi}_{ox}
\]

(19)

which leads to:

\[
\varepsilon \Delta \tilde{\psi} - \tilde{\psi} = - \tilde{C}
\]

(20)

A similar treatment, applied to the electron continuity equation results in:

\[
\nabla \cdot \mu (\varepsilon \tilde{\psi} \nabla \tilde{\eta} - \tilde{\psi}_0) + (\varepsilon \tilde{\psi} - \tilde{\psi}_0) \nabla \tilde{\eta}_0 = \tilde{R}
\]

(21)

Which is equivalent to:

\[
\nabla \cdot \mu (\varepsilon \tilde{\psi} \nabla \tilde{\eta}) = \tilde{R}
\]

where

\[
\tilde{R} = \tilde{R} - \frac{\partial}{\partial x} \mu (\varepsilon \tilde{\psi} - \tilde{\psi} \tilde{\eta} - \tilde{\psi}_0)
\]

(22)
Numerical results

A standard control-volume finite difference solution of the 2D device equations has been coded. This fully numerical solver is used for verification and comparison purposes. The hybrid method was then coded in the form of iterations between outer and inner solutions. The inner solution determines the boundary conditions for the outer potential at the depletion layer. Once this outer solution is numerically computed, the potential drop across the channel determines the channel conductivity for the inner problem. The remarkable property of this scheme is that its accuracy improves as the channel becomes narrower. The standard numerical solution runs into more difficulties under these conditions. In addition to the saving achieved by the coarser grid requirements, it turns out that the hybrid method does not suffer from an excessive number of Gummel iterations, which are needed by the fully numerical solution.

The device in Figure 1 on page 2 has been discretized and solved on a Cartesian grid. Varying levels of refinement were used in the $y$ direction. In the absence of a "true" solution it was assumed that the solution on the finest (20x40) grid is the most accurate. The comparison results, for 2 levels of bulk doping are presented in Table 1. Gate to substrate voltage for both simulations are $V_g = 2$. It can be observed that as the doping level increases the hybrid solution converges more easily, while the fully numerical solutions need a finer grid. This trend represents the fact that steeper layers require larger discretization grid, but their analytic approximation is more accurate.

| Table 1. Solution time for a MOSFET at low-current conditions (sec.) |
|---------------|---------------|---------------|---------------|---------------|---------------|
| grid | $N_A = 10^{15}$ | $N_A = 10^{16}$ | % error | time | % error | time |
| 20x10 | 83 | 2785 | 95 | 2296 | |
| 20x20 | 31 | 6604 | 500 | 5213 | |
| 20x30 | 0.7 | 11016 | 7.5 | 8815 | |
| 20x40 | 0 | 15960 | 0 | 12207 | |
| hybrid | 3 | 688 | 4.3 | 566 | |
Figure 5. The potential boundary layer of a MOSFET device.
References


