LOD-FDTD Method for Physical Simulation of Semiconductor Devices

R. Mirzavand, A. Abdipour, G. Moradi
Electrical Engineering Department
Amirkabir University of Technology
Tehran, Iran
rmirzavand@aut.ac.ir

W.H.A. Schilders
Department of Mathematics and Computer Science
Eindhoven University of Technology
Eindhoven, The Netherlands

M. Movahhedi
Electrical Engineering Department
Shahid Bahonar University of Kerman
Kerman, Iran

Abstract—**This paper describes a locally one-dimensional finite-difference time domain method for the two-dimensional time-dependent simulation of semiconductor devices. This approach leads to significant reduction of the semiconductor simulation time. We can reach over 80% reduction in the simulation time by using this technique while maintaining the same degree of accuracy achieved using the conventional approach. As the first step in the performance investigation, we use the electrons flow equations in the absence of holes and recombination in this paper.**

Keywords- LOD-FDTD; Semiconductor Devices; Drift-Diffusion Model; Physical Simulation

I. INTRODUCTION

Recently, a new implicit method, called the locally-one-dimensional finite-difference time-method (LOD-FDTD), to solve Maxwell's curl equations has been introduced [1]-[3]. This method is an attractive alternative to the standard FDTD due to its unconditional stability with moderate computational overhead and also presents a better computational efficiency than the traditional ADI-FDTD. The unconditional stability means that the LOD-FDTD is free of the Courant–Friedrich–Levy (CFL) stability restraint, allowing any choice of Δt for a stable solution. Similar to ADI-FDTD, the LOD-FDTD can be particularly useful for problems involving devices with fine geometric features that are much smaller than the wavelengths of interest [4].

Many different approaches to the simulation of semiconductor devices have been developed in the past. All of these techniques are fundamentally dependent upon the solution of the Poisson equation along with the basic carrier transport equations. In this paper, the semiconductor analysis is based on the time-domain drift-diffusion method (DDM) [5]. The set of DDM equations contains the Poisson equation and the carrier transport equations, obtained by splitting the Boltzmann transport equation (BTE) into its first two moments. The DDM model assumes that the carrier temperature is equal to the semiconductor lattice temperature. Therefore, the carrier velocity is dependent on the electric field only. In comparison to other, more rigorous techniques for numerical modeling of semiconductor devices, the DDM is a relatively simple technique with better convergence of the algorithm and shorter computational times. Therefore, it is more suitable for use by a design engineer.

This paper presents a semi-implicit numerical method to solve the DDM equation based on LOD-FDTD scheme. This allows using a larger time-step size that leads significantly to CPU time reduction while maintaining the same degree of accuracy achieved using the conventional approach.

II. TRANSISTOR PHYSICAL MODEL

The semiconductor models used are based on the moments of Boltzmann's transport equations obtained by integration over the momentum space. Three equations need to be solved together with Poisson's equation in order to get the quasi-static characteristics of the transistor. This system of coupled highly nonlinear partial differential equations contains current continuity, energy conservation and momentum conservation equations [5]. The solution of this system of partial differential equations represents the complete hydrodynamic model. Simplified models are obtained neglecting some terms in momentum equation. One of these simplified models is drift-diffusion model (DDM). In this paper we simulate MESFET as microwave/mm transistor that is a unipolar device. For this device, the equations to be solved in the drift-diffusion model are

$$\nabla^2\phi = -\rho/\varepsilon = -q(N_d^+ - n)/(\varepsilon_0\varepsilon_r), \tag{1}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot\vec{J}_n = \frac{1}{q}\left(\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y}\right), \tag{2}$$

$$\vec{J}_n = qn\mu_n(\vec{E}, N_d)\vec{E} + qD_n(\vec{E}, N_d)\nabla n, \tag{3}$$

$$\vec{E} = -\nabla\phi. \tag{4}$$

This work was supported in part by Iran Telecommunication Research Center (ITRC).

where $\mu_n = (\mu_0 + v_s E^3 / E_s^4)/(1 + E^4 / E_s^4)$ and $D_n = \mu_n K_B T/q$. In the above equations, ϕ is the potential, N_d^+ is the doping profile, n is the electron concentration, and μ_n and D_n are the mobility and the diffusion coefficient, respectively.

To have a numerically stable estimation of the electron concentration between nodes, we use the following equation [6]-[7] in the x and y directions

$$n(c) = \{1 - g(c,\phi)\}\, n(a) + g(c,\phi) n(b)\ ; \quad c \in [a,b] \tag{5}$$

where $g(c,\phi) = \{1\text{-}\exp(CV)\}/\{1\text{-}\exp(V)\}$, $V = (\phi_b\text{-}\phi_a)q/KT$, and $C = (c\text{-}a)/(b\text{-}a)$. Equation (1) can be discretized using the carrier concentration $n_{i,j}$ at $t = k\,\Delta t$ as the following

$$\frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{(\Delta x^2)} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{(\Delta y^2)} = -\frac{q}{\varepsilon}(N_d^+ - n_{i,j}^k). \tag{6}$$

By applying the LOD principle [8], the computation of (2) for the FDTD solution marching from the k^{th} time-step to the $(k + 1)^{\text{th}}$ time-step is broken up into two computational sub-advancements: the advancement from the k^{th} time-step to the $(k + 1/2)^{\text{th}}$ time-step and the advancement from the $(k + 1/2)^{\text{th}}$ time-step to the $(k + 1)^{\text{th}}$ time-step. More specifically, the two substeps are as follows.

Step 1) For the first half-step, i.e., at the $(k + 1/2)^{\text{th}}$ time step, the first partial derivative on the right-hand side (RHS) of (1), $\partial J_x/\partial x$, is replaced with the average of explicit and implicit difference approximation of its known and unknown pivotal values at the k^{th} and $(k + 1/2)^{\text{th}}$ time step, while the second partial derivatives on the RHS, $\partial J_y/\partial y$, is removed. Using the first-order upwind scheme for spatial derivatives,

$$v_i \frac{d}{dx}[f_i] = \begin{cases} v_i (f_i - f_{i-1})/\Delta x & \text{if } v_i \geq 0, \\ v_i (f_{i+1} - f_i)/\Delta x & \text{if } v_i < 0. \end{cases} \tag{7}$$

yields the following equation,

$$\begin{aligned}
&-\left[\frac{\Delta t D_{i+1j}}{2\Delta x^2} + \frac{\Delta t\, \mu_{i+1j}\alpha_{xi+1}(|E_x| + E_x)}{4\Delta x}\right] n_{i+1,j}^{k+1/2} \\
&+\left[1 + \frac{\Delta t D_{ij}}{\Delta x^2} + \frac{\Delta t\, \mu_{ij}(\alpha_{xi+1} + \alpha_{xi})|E_x|}{4\Delta x} + \frac{\Delta t\, \mu_{ij}}{2}\frac{\partial^2\phi}{\partial x^2}\right] n_{i,j}^{k+1/2} \\
&-\left[\frac{\Delta t}{2\Delta x^2} D_{i-1j} + \frac{\Delta t\, \mu_{i-1j}\alpha_{xi}(|E_x| - E_x)}{4\Delta x}\right] n_{i-1,j}^{k+1/2} \\
&=\left[\frac{\Delta t}{2\Delta x^2} D_{i+1j} + \frac{\Delta t\, \mu_{i+1j}\alpha_{yj+1}(|E_x| + E_x)}{4\Delta x}\right] n_{i+1,j}^{k} + \\
&\left[1 - \frac{\Delta t}{\Delta x^2} D_{ij} - \frac{\Delta t\, \mu_{ij}(\alpha_{xj+1} + \alpha_{xj})|E_x|}{4\Delta x} + \frac{\Delta t\, \mu_{ij}}{2}\frac{\partial^2\phi}{\partial x^2}\right] n_{i,j}^{k} + \\
&\left[\frac{\Delta t}{2\Delta x^2} D_{i-1j} + \frac{\Delta t\alpha_{x-1j}(|E_x| - E_x)}{4\Delta x}\right] n_{i-1,j}^{k}.
\end{aligned} \tag{8}$$

where

$$\alpha_{xi} = \frac{V_{xi}/2}{\Delta x \cdot \sinh(V_{xi}/2)} \text{ and } V_{xi} = \frac{\phi_{i,j} - \phi_{i-1,j}}{KT/q}.$$

Step 2) For the second half time-step, i.e., at $(k + 1)^{\text{th}}$ time step, the second term on the RHS, $\partial J_y/\partial y$, is replaced with the average of explicit and implicit difference approximation of its known and unknown pivotal values at the $(k + 1/2)^{\text{th}}$ and $(k + 1)^{\text{th}}$ time step, while the second partial derivatives on the RHS, $\partial J_x/\partial x$, is discarded. Using the first-order upwind scheme for spatial derivatives, the following equation cab be derived,

$$\begin{aligned}
&-\left[\frac{\Delta t}{2\Delta y^2} D_{ij+1} + \frac{\Delta t\, \mu_{ij+1}\alpha_{yj+1}(|E_y| + E_y)}{4\Delta y}\right] n_{i,j+1}^{k+1} \\
&+\left[1 + \frac{\Delta t}{\Delta y^2} D_{ij} + \frac{\Delta t\, \mu_{ij}(\alpha_{yj+1} + \alpha_{yj})|E_y|}{4\Delta y} + \frac{\Delta t\, \mu_{ij}}{2}\frac{\partial^2\phi}{\partial y^2}\right] n_{i,j}^{k+1} \\
&-\left[\frac{\Delta t}{2\Delta y^2} D_{ij-1} + \frac{\Delta t\, \mu_{ij-1}\alpha_{yj}(|E_y| - E_y)}{4\Delta y}\right] n_{i,j-1}^{k+1} \\
&=\left[\frac{\Delta t D_{ij+1}}{2\Delta y^2} + \frac{\Delta t\, \mu_{ij+1}\alpha_{yi+1}(|E_y| + E_y)}{4\Delta y}\right] n_{i,j+1}^{k+1/2} \\
&+\left[1 - \frac{\Delta t D_{ij}}{\Delta y^2} - \frac{\Delta t\, \mu_{ij}(\alpha_{yi+1} + \alpha_{yi})|E_y|}{4\Delta y} + \frac{\Delta t\, \mu_{ij}}{2}\frac{\partial^2\phi}{\partial y^2}\right] n_{i,j}^{k+1/2} \\
&+\left[\frac{\Delta t}{2\Delta y^2} D_{ij-1} + \frac{\Delta t\, \mu_{ij-1}\alpha_{yi}(|E_y| - E_y)}{4\Delta y}\right] n_{i,j-1}^{k+1/2}.
\end{aligned} \tag{9}$$

where

$$\alpha_{yi} = \frac{V_{yi}/2}{\Delta y \cdot \sinh(V_{yi}/2)} \text{ and } V_{yi} = \frac{\phi_{i,j} - \phi_{i,j-1}}{KT/q}.$$

Therefore the system of linear equations can be obtained which are symmetric and tridiagonal, and thus cheap to solve by methods like Choleski decomposition [9]. Fig. 1 shows flowchart of the sequence of LOD-FDTD scheme for DDF model.

III. Simulation Results

The transistor considered in this simulation is a 0.6 μm gate MESFET. Fig. 2 presents the conventional 2-D structure used for simulation. Here, a uniform mesh that covers the 2-D cross section of the MESFET is used (65×32).

The time-step size in the explicit methods for the semiconductor equations is a function of the average carrier

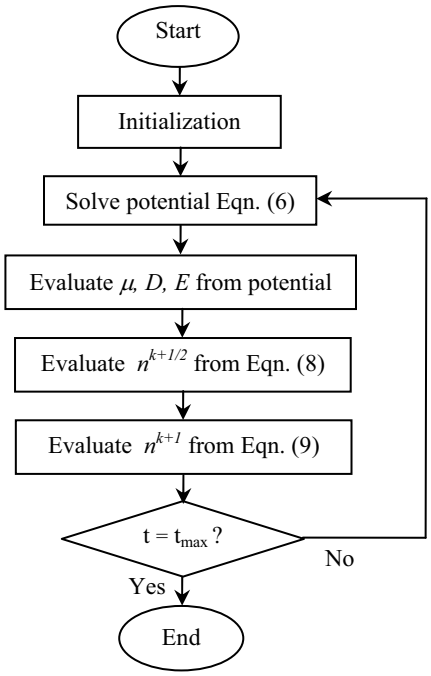

Figure 1. Flowchart of the sequence of LOD-FDTD scheme for DDF model.

velocity v_d and the spatial step to comply with the following CFL condition for stability and minimizing numerical dispersion [10],

$$v_d \Delta t \le \left[\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right]^{-1/2} \qquad (10)$$

For the given cell size, the time-step sizes is about 10^{-15} s for conventional FDTD method. As the LOD-FDTD is unconditionally stable, a greater time-step size can be used for it. Here, Δt will be increased by a factor of 100.

The device is biased and the dc parameter distributions (potential and carrier density) are obtained by solving the drift-diffusion model. The device is biased to V_{ds}= *2 V* and V_{gs}= *-0.5 V*. The state of the MESFET under dc steady state is represented by the distribution of potential and carrier density. It is to be noted that Dirichlet boundary conditions are used at the electrodes while Neumann boundary conditions are used at the other walls.

Fig. 3 shows the potential and carrier density distributions obtained using the LOD-FDTD scheme. A comparison between results of different algorithms is provided in Figs. 4 and 5. It is significant to indicate that the LOD-FDTD method gives precisely the same results obtained when the FDTD method is used whereas in the case of using LOD-FDTD scheme, the CPU time is reduced by 83% with a maximum numerical dispersion error of 0.001%. For this 2D problem, the ADI and LOD approaches have a very close performance.

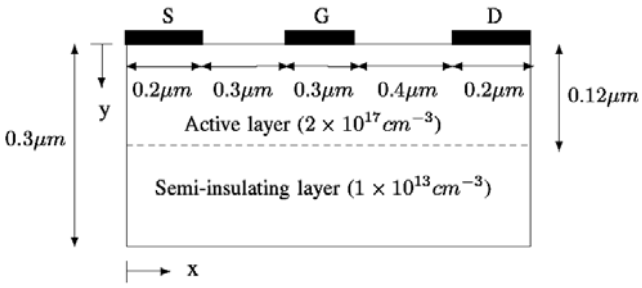

Figure 2. Cross section of the simulated MESFET.

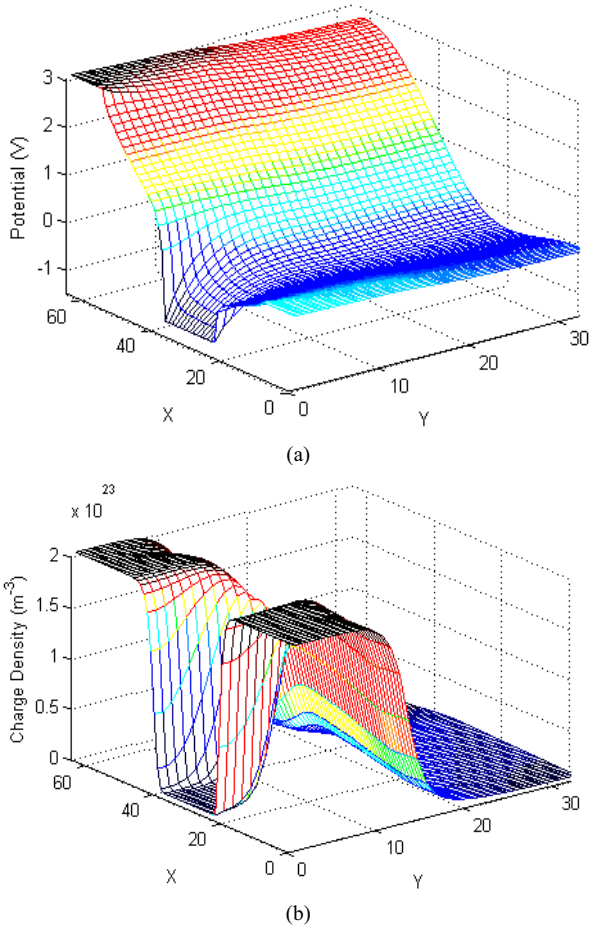

Figure 3. Sample DC results obtained using the proposed algorithm, (a) Potential distribution, (b) Carrier density distribution.

IV. CONCLUSION

This work proposed a numerical method for simulation of time dependent drift-diffusion model of semiconductor devices in two dimensions. Using the LOD-FDTD method to solve semiconductor equations allows increasing the time-step size by a factor of 100 and obtaining 83% reduction in the simulation time with a negligible error.

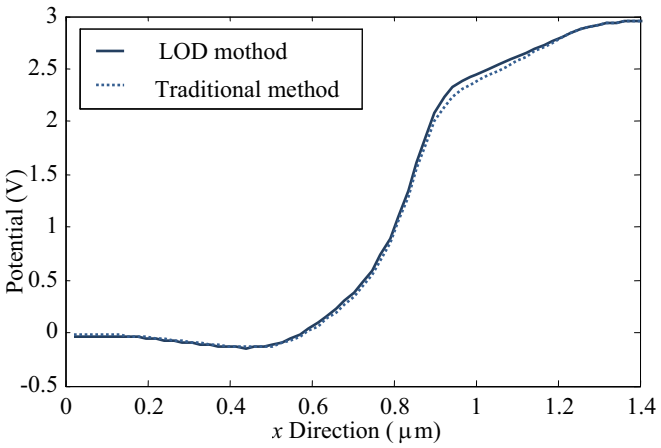

Figure 4. Potential distribution across the x direction for $y = 0.09$ μm.

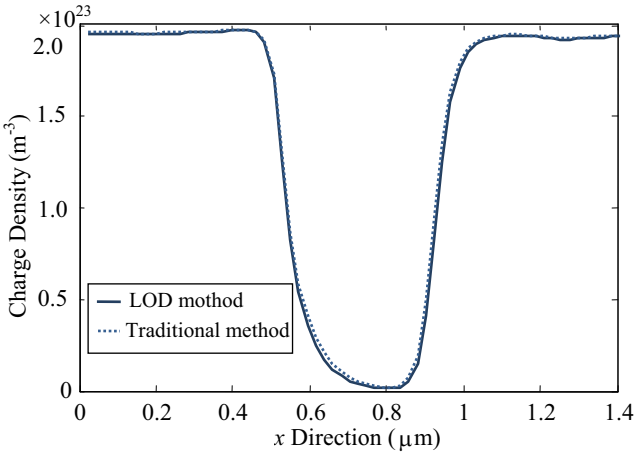

Figure 5. Charge Density (n) across the x direction for $y = 0.09$ μm.

REFERENCES

[1] J. Lee and B. Fornberg, "Some unconditionally stable time stepping methds for the 3D Maxwell," *J. Comput. Appl. Math.*, vol. 158., pp. 484-505, 2004.

[2] J. Shibayama, M. Muraki, J. Yamauchi and H. Nakano, "Efficient implicit FDTD algorithm based on locally one-dimensional scheme," *Electron. Lett.*, vol. 41, no. 19, Sept. 2005.

[3] Q.F. Liu, Z. Chen, and W.Y. Yin, "An Arbitrary-Order LOD-C Method and its Stability and Numerical Dispersion," *IEEE Trans. On Ante. and Propag.*, vol. 57, no. 8, Aug. 2009.

[4] M. Movahhedi, A. Abdipour, "Efficient Numerical Methods for Simulation of High-Frequency Active Devices," IEEE Trans. Microw. Theory and Tech., vol. 54, no. 6, pp. 2636-2645, June 2006.

[5] Y. K. Feng, and A. Hintz, "Simulation of sub-micrometer GaAs MESFET's using a full dynamic transport model," *IEEE Trans. Electron Devices*, vol. 35, pp. 1419–1431, September 1988.

[6] D. L. Scharfetter and H. K. Gummel, "C signal analysis of a Silicon Read diode oscillator," *IEEE Trans. Electron Devices*, vol. ED-16, pp. 64–77, 1969.

[7] H. K. Gummel, "A self-consistent iterative scheme for one-dimensional steady state transistor calculation," *IEEE Trans. Electron Devices*, vol. ED-11, pp. 455–465, 1964.

[8] K. W. Morton, and D. F. Mayers, *Numerical Solution of Partial Differential Equations*, Second Edition, New York: Cambridge University Press, 2005.

[9] D. Bau III, and L.N. Trefethen, Numerical linear algebra, Philadelphia: Society for Industrial and Applied Mathematics, 1997.

[10] K. Tomizawa, *Numerical Simulation of Submicron Semiconductor Devices*, Norwood, MA: Artech House, 1993.