FDLTD method for the Physical Simulation of Microwave FET Transistor

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Abstract: *This paper describes an new application of weighted Laguerre polynomial functions to produce a unconditionally stable Finite-Difference Laguerre-Time-domain (FDLTD) scheme for simulation of the Drift-Diffusion Model (DDM) of microwave active devices. The unconditionally stability of FDLTD method leads to a significant reduction in the simulation time. For example, when 100 weighted Laguerre polynomial functions is used, FDLTD is 5 times faster than conventional FDTD method while they have the same degree of accuracy.*

Keywords: Microwave FET Transistor, Semiconductor Device, finite-difference Laguerre time-domain (FDLTD), Drift-Diffusion Model.

1. Introduction

Fundamentally, all of semiconductor's physical simulation techniques depend on the solution of Poisson equation along with the basic carrier transport equations [1, 2]. In this paper, the analysis of microwave FET transistor is based on the time-domain drift-diffusion model (DDM) [3]. The set of DDM equations contains Poisson equation and the carrier transport equations, obtained by splitting Boltzmann transport equation (BTE) into its first two moments. DDM assumes that the carrier velocity is depended on the electric field only. Therefore, DDM is a simple technique with better convergence and shorter computational time in comparison to the other more rigorous semiconductors' numerical modelling. Thus, this simple modelling process is more suitable for use by a design engineer in the first step of the transistor's design. While in the next steps, one can use a more accurate model.

Recently a new unconditionally stable scheme for simulation of the time-domain Maxwell's equations was introduced based on the Laguerre polynomials [4]. This method is a marching-on-in-degree method instead of marching-on-in-time method and therefore the stability is no longer affected by the time step size [4]-[8]. The time step is used only to calculate the coefficients of source's Laguerre domain representation. As the transformation of the time domain source to the Laguerre domain is done only at the start of the computations, selecting a smaller value for Δt can improve the accuracy of solution to a desired value without significant additional computation load. Therefore, Laguerre based method may be computationally much more efficient than the FDTD methods [4]-[6].

In the first part of this paper, we describe the Laguerre domain representation of a function. In the second part, a new unconditionally stable FDLTD method is presented for the two-dimensional time-dependent simulation of nonlinear drift-diffusion model. The FDLTD method allows simulating the whole desired time in only one shot without stability failures while the accuracy is still acceptable. In the last part, we use the proposed method to analyse an example microwave MESFET transistor. Compared with the conventional FDTD method for a desired accuracy, the new unconditionally stable method is 5 times faster in our example when 100 weighted Laguerre polynomial functions is used.

2. Laguerre Transform

Laguerre polynomials are defined by the Rodrigues formula [9],

$$L_p(t) = \frac{e^t}{p!}\frac{d^p}{dt^p}\left(e^t t^p\right);\ p = 0,1,\ldots \tag{1}$$

or recursively as,

$$L_0(t) = 1, \tag{2}$$

$$L_1(t) = 1 - t, \tag{3}$$

$$pL_p(t) = (2p - 1 - t)L_{p-1}(t) - (p-1)L_{p-2}(t);\ p \geq 2 \tag{4}$$

Defining the weighted Laguerre functions [6], $\psi_p(t)$, as

$$\psi_p(t) = e^{-t/2}L_p(t), \tag{5}$$

make them orthogonal to each other over [0, ∞),

$$\int_0^\infty \psi_p(t)\psi_q(t)dt = \begin{cases} 0 & p \neq q \\ 1 & p = q \end{cases} \tag{6}$$

Therefore, an approximation of a function $u(\mathbf{r}, t)$ may be written as a linear combination of N modified Laguerre functions,

$$u(\mathbf{r},t)=\sum_{p=0}^{N}u^{p}(\mathbf{r})\psi_{p}(\bar{t});\ \bar{t}=s\cdot t \tag{7}$$

where $\mathbf{r} = x\boldsymbol{a}_x + y\boldsymbol{a}_y + z\boldsymbol{a}_z$ is the position vector, s is a scaling factor to increase the time scale to the order of second and $u^{p}(\mathbf{r})$ are the spatial domain expansion coefficients, given by

$$u^{p}(\mathbf{r})=\int_{0}^{\infty}\psi_{p}(\bar{t})u(\mathbf{r},\bar{t})d\bar{t} \tag{8}$$

The first-order partial derivative of function $u(\mathbf{r},t)$, respect to the time, can be expressed as [9]:

$$\frac{\partial u(\mathbf{r},t)}{\partial t}=s\sum_{p=0}^{N}u^{pp}(\mathbf{r})\psi_{p}(\bar{t}) \tag{9}$$

where

$$u^{pp}(\mathbf{r})=0.5u^{p}(\mathbf{r})+\sum_{k=0,p\neq 0}^{p-1}u^{k}(\mathbf{r}) \tag{10}$$

3. Transistor Physical Model in Laguerre domain

The employed semiconductor models 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 [3]. 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 the drift-diffusion model (DDM) [3]. In this paper, we simulate a MESFET as a microwave transistor that is a unipolar device. For this device, the equations to be solved in the drift-diffusion model are,

$$\frac{\partial n}{\partial t}=\frac{1}{q}\nabla\cdot\vec{J} \tag{11}$$

$$\vec{J}=-q\,\mu_{n}(\vec{E},N_{d})n\nabla\varphi+qD_{n}(\vec{E},N_{d})\nabla n \tag{12}$$

$$\nabla^{2}\varphi=-\frac{q}{\varepsilon_{0}\varepsilon_{r}}(N_{d}-n) \tag{13}$$

where φ is potential, $E = -\nabla\varphi$, N_d is doping profile, n is the electron (carrier) density, μ_n and $D_n = \mu_n K_B T/q$ are mobility and diffusion coefficients, respectively. The electron mobility has been considered as a function of doping and electric field [10]:

$$\mu_{n}(E,N_{d})=\frac{\mu_{0}+(v_{s}/E)(E/E_{s})^{4}}{1+(E/E_{s})^{4}} \tag{14}$$

while low-field mobility μ_0, saturation velocity v_s, and critical field E_s (for the onset of negative differential mobility) are functions of doping N_d.

According to (7), the approximation of all components in DDM can be expanded as,

$$n(\mathbf{r},t)=\sum_{p=0}^{N}n^{p}(\mathbf{r})\psi_{p}(\bar{t}) \tag{15}$$

$$\varphi(\mathbf{r},t)=\sum_{p=0}^{N}\varphi^{p}(\mathbf{r})\psi_{p}(\bar{t}) \tag{16}$$

$$J_{r}(\mathbf{r},t)=\sum_{p=0}^{N}J_{r}^{p}(\mathbf{r})\psi_{p}(\bar{t});\ r=x,y \tag{17}$$

where $n^p(\mathbf{r})$, $\varphi^p(\mathbf{r})$, $J_x^p(\mathbf{r})$, and $J_y^p(\mathbf{r})$ are unknown coefficients to be determined. Subtituting (15)-(17) into (11)-(13), Laguerre domain equatons are obtained as,

$$s\sum_{p=0}^{N}[0.5n^{p}+\sum_{k=0,p>0}^{p-1}n^{k}]\psi_{p}(\bar{t})=\frac{1}{q}\sum_{p=0}^{N}[\frac{\partial J_{x}^{p}}{\partial x}+\frac{\partial J_{y}^{p}}{\partial y}]\psi_{p}(\bar{t}) \tag{18}$$

$$\sum_{p=0}^{N}J_{r}^{p}\psi_{p}(\bar{t})=-q\mu_{n}[\sum_{p=0}^{N}n^{p}\psi_{p}(\bar{t})][\sum_{p=0}^{N}\frac{\partial\varphi^{p}}{\partial r}\psi_{p}(\bar{t})]+qD_{n}\sum_{p=0}^{N}\frac{\partial n^{p}}{\partial r}\psi_{p}(\bar{t});\ r=x,y \tag{19}$$

$$\sum_{p=0}^{N}[\frac{\partial^{2}\varphi^{p}}{\partial x^{2}}+\frac{\partial^{2}\varphi^{p}}{\partial y^{2}}]\psi_{p}(\bar{t})=\frac{-q[N_{d}-\sum_{p=0}^{N}n^{p}\psi_{p}(\bar{t})]}{\varepsilon_{0}\varepsilon_{r}} \tag{20}$$

The products in (19) can simplified as,

$$\begin{aligned}&[\sum_{p=0}^{N}n^{p}\psi_{p}][\sum_{p=0}^{N}\frac{\partial\varphi^{p}}{\partial r}\psi_{p}]\\&=\sum_{q=0}^{N}\sum_{k=0}^{N}\left[n^{q}\frac{\partial\varphi^{k}}{\partial r}\psi_{q}\psi_{k}\right]\\&=\sum_{p=0}^{N}\left[\sum_{q=0}^{N}\sum_{k=0}^{N}a_{p,q,k}n^{q}\frac{\partial\varphi^{k}}{\partial r}\right]\psi_{p}\\&=\sum_{p=0}^{N}A_{r}^{p}\psi_{p}\end{aligned} \tag{21}$$

multiplying both side of (18)-(20) by $\psi_m(\bar{t})$, integrating them in range $\bar{t}=[0,\infty)$ and using (6), we get a set of (N+1) boundary value problems as,

$$\left[0.5n^{m}+\sum_{k=0,m>0}^{m-1}n^{k}\right]=\frac{1}{q}\left[\frac{\partial J_{x}^{m}}{\partial x}+\frac{\partial J_{y}^{m}}{\partial y}\right] \tag{22}$$

$$J_{r}^{m}=-q\,\mu_{n}A_{r}^{m}+qD_{n}\frac{\partial n^{m}}{\partial r}\quad;\ r=x,y \tag{23}$$

$$\frac{\partial^{2}\varphi^{m}}{\partial x^{2}}+\frac{\partial^{2}\varphi^{m}}{\partial y^{2}}=\frac{-q}{\varepsilon_{0}\varepsilon_{r}}\left[N_{d}^{m}-n^{m}\right] \tag{24}$$

where

$$\begin{aligned}N_{d}^{m}&=N_{d}^{m}(\mathbf{r})=\int_{0}^{\infty}N_{d}(\mathbf{r})\psi_{m}(\bar{t})d\bar{t}\\&=N_{d}(\mathbf{r})\int_{0}^{\infty}\psi_{m}(\bar{t})d\bar{t}\\&=2N_{d}(\mathbf{r})(-1)^{m}\end{aligned} \tag{25}$$

for m = 0, 1, … N. Now the solution domain is discretized by two sets of scattered nodes, one defining the scalar quantity at the nodal points and the other defining the vector quantity positioned at the midpoint of the cells of nodal points, similar to the conventional

FDTD method. Therefore using central difference scheme in the space domain, (22)-(25) are discretized as,

$$n_{i,j}^{m} = \sum_{k=0,m>0}^{m-1} n_{i,j}^{k} + 2\left[J_{x\,i,j}^{m} - J_{x\,i-1,j}^{m}\right]/qs\Delta x_i + 2\left[J_{y\,i,j}^{m} - J_{y\,i,j-1}^{m}\right]/qs\Delta y_j \quad (26)$$

$$J_{x\,i,j}^{m} = -q\mu_{n\,i,j}\sum_{q=0}^{N}\sum_{k=0}^{N}\left[a_{m,q,k}\,n^{q}(\varphi_{i+1,j}^{k} - \varphi_{i,j}^{k})/\Delta x_i\right] + qD_{n\,i,j}(n_{i+1,j}^{m} - n_{i,j}^{m})/\Delta x_i \quad (27)$$

$$J_{y\,i,j}^{m} = -q\mu_{n\,i,j}\sum_{q=0}^{N}\sum_{k=0}^{N}\left[a_{m,q,k}\,n^{q}(\varphi_{i,j+1}^{k} - \varphi_{i,j}^{k})/\Delta y_i\right] + qD_{n\,i,j}(n_{i,j+1}^{m} - n_{i,j}^{m})/\Delta y_i \quad (28)$$

$$\frac{(\varphi_{i+1,j}^{m} - 2\varphi_{i,j}^{m} + \varphi_{i-1,j}^{m})}{\Delta x^{2}} + \frac{(\varphi_{i,j+1}^{m} - 2\varphi_{i,j}^{m} + \varphi_{i,j-1}^{m})}{\Delta y^{2}} = \frac{-q}{\varepsilon_0\varepsilon_r}\left[N_{d\,i,j}^{m} - n_{i,j}^{m}\right] \quad (29)$$

for $i = 1, 2, \ldots N_x$ and $j = 1, 2, \ldots N_y$ where N_x and N_y are total number of grids in x and y directions, respectively. Considering Dirichlet and Neumann boundary conditions as,

$$\frac{\partial n}{\partial x} = 0, J_x = 0, \frac{\partial J_y}{\partial x} = 0, \frac{\partial \varphi}{\partial x} = 0 \quad \text{at } x = \{0, x_{\max}\}$$
$$\frac{\partial n}{\partial y} = 0, J_y = 0, \frac{\partial J_x}{\partial y} = 0, \frac{\partial \varphi}{\partial y} = 0 \quad \text{at } y = \{0, y_{\max}\} \quad (32)$$
$$\varphi = v_{gs}(t) \quad \text{at } Gate$$

the following equations are obtained in the Laguerre domain

$$n_{1,j}^{m} = n_{2,j}^{m}, n_{N_x,j}^{m} = n_{N_x-1,j}^{m},$$
$$\varphi_{1,j}^{m} = \varphi_{2,j}^{m}, \varphi_{N_x,j}^{m} = \varphi_{N_x-1,j}^{m},$$
$$J_{x1,j}^{m} = J_{xN_x,j}^{m} = 0, J_{y1,j}^{m} = J_{y2,j}^{m}, J_{yN_x,j}^{m} = J_{yN_x-1,j}^{m},$$
$$n_{i,1}^{m} = n_{j,2}^{m}, n_{i,N_y}^{m} = n_{i,N_y-1}^{m}, \quad (33)$$
$$\varphi_{i,1}^{m} = \varphi_{i,2}^{m}, \varphi_{i,N_y}^{m} = \varphi_{i,N_y-1}^{m},$$
$$J_{yi,1}^{m} = J_{yi,N_y}^{m} = 0, J_{xi,1}^{m} = J_{xi,2}^{m}, J_{xi,N_y}^{m} = J_{xi,N_y-1}^{m},$$
$$\varphi_{i,1}^{m} = \int_0^{T_d} v_{gs}(\bar{t})\psi(\bar{t})d(\bar{t}); \; N_1 \le i \le N_2$$

where T_d is the truncated time for numerical calculation of infinite integral and $V_{gs}(t)$ is the applied AC voltage to the gate. In (36), N_1 and N_2 are the grid's number for start and end of gate in x direction, respectively.

The system of $4\times(N+1) \times N_x \times N_y$ equations (26)-(39), together with boundary conditions (33), form a nonlinear set of equations for unknowns $\{X^m\} = \{n^m, J_x^m, J_y^m, \varphi^m\}$. As this is a large-scale nonlinear system, we need a method with minimal memory requirements. The recently presented method, Derivative-free Spectral Algorithm for Nonlinear Equations (DF-SANE) [11] is a good candidate for this purpose.

Note that the stability is no longer affected by the time step size. In FDLTD the time step is used only to calculate the Laguerre coefficients in (33).

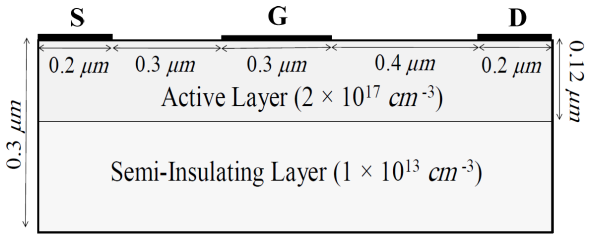

Fig. 1: Cross section of the simulated MESFET

4. Simulation Results

In order to demonstrate the performance of the proposed approach, the microwave GaAs MESFET transistor shown in Fig. 1 is considered. Here, a uniform mesh that covers the 2-D cross section of the MESFET is used with 65×32 cells. Initially, 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 DC distributions of parameters are obtained by solving the physical model equations. The state of the MESFET under dc steady state is represented by the distribution of potential and carrier density.

Fig. 2 shows the calculated potential at an example point in the simulation domain by FDTD and FDLTD algorithms. It can be seen in Fig. 3 that 100 modified Laguerre functions is enough for this example to reach the stable results.

Fig. 4 illustrates the carrier density distributions. It is significant to indicate that the proposed algorithm gives precisely the same results as the FDTD method's results.

The FDLTD simulation contains 100 modified Laguerre functions with $s = 2.5 \times 10^{14}$. In this case, FDLTD with DF-SANE is 5 times faster than the conventional FDTD method while they have the same degree of accuracy in results.

5. Conclusion

This work proposed a new unconditionally stable numerical method for the simulation of time dependent drift-diffusion model of semiconductor devices in two dimensions. The method is based on the weighted Laguerre polynomial functions which can leads to a significant reduction in the simulation time without accuracy loss.

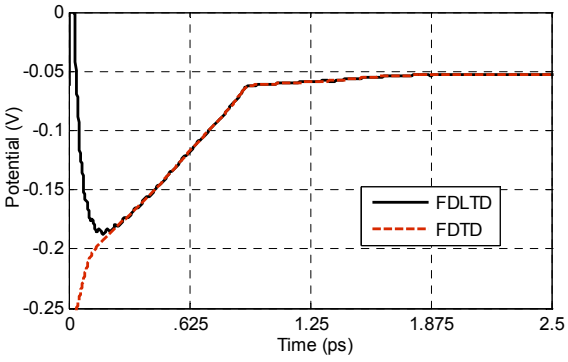

Fig. 2: Potential at (x,y) =(0.83, 0.09) μm

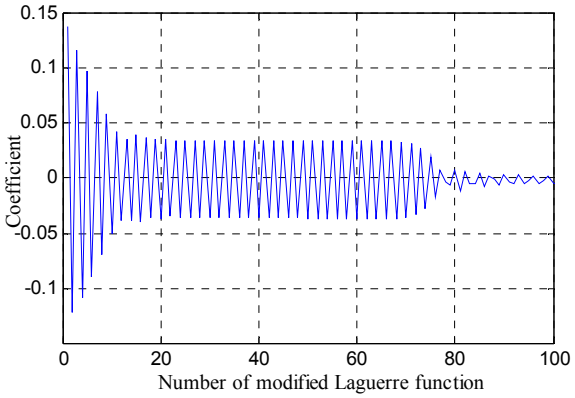

Fig. 3: Coefficients of potential at (x,y) =(0.83, 0.09) μm in the Laguerre domain

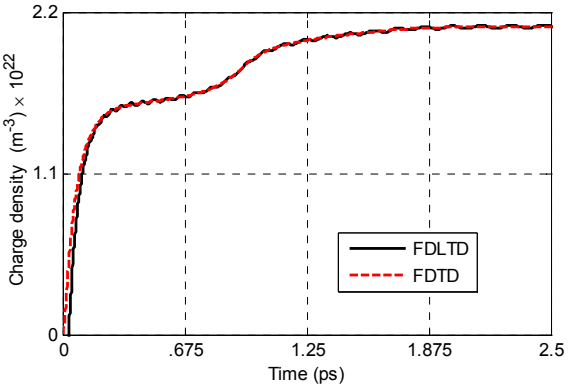

Fig. 4: Charge density at (x,y) =(0.83, 0.09) μm

Acknowledgements

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

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