A Meshless Method for Physical Simulation of Semiconductor Devices

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***Abstract* — This paper describes a meshless method for the two-dimensional time-dependent simulation of semiconductor devices. In this method the solution is approximated using global radial basis functions (RBF) and distributed quasi-random points can be used. This allows the computation of problems with complex-shaped boundaries and forming fine and coarse points abundance in locations where variable solutions change rapidly and slowly, respectively. As the first step in the performance investigation, we use the electrons flow equations in the absence of holes and recombination in this paper.**

***Index Terms* — Drift-Diffusion Model, meshless (meshfree), Poisson's equation, radial basis functions (RBF), semiconductor devices.**

I. Introduction

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). 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.

Recently, considerable effort has been devoted to the development of meshless methods to find the numeric solution of partial differential equations [1]. In 1990, Kansa introduces a new approach for this kind of problems, where the true solution is approximated for a linear combination of radial basis functions [2]. This method has shown to be more efficient than the traditional methods like, Finite Differences Methods and Finite Element Methods [3, 4]. In this method as the name applies, it does not require any connectivity information, i.e., mesh but only requires nodes to generate shape functions. A big obstacle for radial basis function collocation method is that the companion matrix is generally ill-conditioned, nonsymmetric and full dense matrix, which constrains the applicability of RBFs method to solve large scale problems. Hence, domain decomposition method can provide a way to reduce the computational time and the ill-conditioning of the matrix.

This paper presents a numerical method to solve the DDM equation by approximating directly the solution using global radial basis functions. The method is similar to finite differences but with the advantage of arbitrary point locations. Due to the radial nature of the basis functions used, the schemes also make no distinction regarding the dimension of the problem.

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:

$$\vec{J}_n = qn\mu_n(\vec{E}, N_d)\vec{E} + qD_n(\vec{E}, N_d)\nabla n \qquad (1)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot \vec{J}_n \qquad (2)$$

$$\nabla^2 \varphi = -\frac{q}{\varepsilon_0 \varepsilon_r}(N_d^+ - n) \qquad (3)$$

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where φ is potential, $\vec{E} = -\nabla\phi$, N_d^+ is doping profile, n is the electron (carrier) density, and μ_n is the mobility coefficient and $D_n = \mu_n K_B T / q$. In this work, electron mobility has been considered as a function of doping and electric field:

$$\mu_n(E, N_d) = \frac{\mu_0 + (v_s / E)(E / E_s)^4}{1 + (E / E_s)^4} \qquad (4)$$

The parameters of this equation have been defined in [6].

III. Meshless Method Based on RBF

The approximation of a function $u^h(\mathbf{x})$, using radial basis functions, may be written as a linear combination of N radial functions [7],

$$u^h(\mathbf{x}) \simeq \sum_{i=1}^{N} a_i \phi(\mathbf{x}, \mathbf{x}_i) = \Phi^T \mathbf{a} \quad ; \mathbf{x} \in R^d \qquad (5)$$

where N is the number of data points, $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ is the vector position, d is the dimension of the problem, a_i's are coefficients to be determined and ϕ is the radial basis function. The coefficients a_i are determined by forcing the interpolation to pass through all the N collocation points, resulting in

$$u^h(\mathbf{x}) = \Phi^T A^{-1} \mathbf{u} = \mathbf{N}(\mathbf{x})\mathbf{u} \qquad (6)$$

where $\mathbf{u} = [u(x_1), u(x_2), \ldots, u(x_N)]^T$,

$$\mathbf{A} = \begin{bmatrix} \Phi(x_1) \\ \Phi(x_2) \\ \vdots \\ \Phi(x_N) \end{bmatrix} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_N) & \phi_2(x_N) & \cdots & \phi_N(x_N) \end{bmatrix} \qquad (7)$$

And the first-order partial derivative of function, respect to the space variables, can be expressed as [7]:

$$\frac{\partial u^h(\mathbf{x})}{\partial x^i} = \mathbf{N}(\mathbf{x})_{,i}\,\mathbf{u} \qquad (8)$$

where

$$\mathbf{N}(\mathbf{x})_{,i} = \Phi_{,i}^T A^{-1} = [\phi_{1,i}(\mathbf{x}), \phi_{2,i}(\mathbf{x}), \ldots, \phi_{N,i}(\mathbf{x})]^T A^{-1} \qquad (9)$$

According to (6), the approximation of all components in DDM can be expanded with the same RBF:

$$n(\mathbf{x}, t) = \mathbf{N}(\mathbf{x})\upsilon(t) \qquad (10)$$

$$\varphi(\mathbf{x}, t) = \mathbf{N}(\mathbf{x})\zeta(t) \qquad (11)$$

$$J_x(\mathbf{x}, t) = \mathbf{N}(\mathbf{x}) j_x(t), J_y(\mathbf{x}, t) = \mathbf{N}(\mathbf{x}) j_y(t) \qquad (12)$$

$$E_x(\mathbf{x}, t) = \mathbf{N}(\mathbf{x}) e_x(t), E_y(\mathbf{x}, t) = \mathbf{N}(\mathbf{x}) e_y(t) \qquad (13)$$

where $\upsilon(t)$, $\zeta(t)$, $j_x(t)$, $j_y(t)$, $e_x(t)$ and $e_y(t)$ are unknown time coefficient vectors to be computed at the collocation nodes. Thus, equations (1) - (3) discretize using (10)-(13) and finite difference approximation for time derivative,

$$\mathbf{N}\upsilon^{k+1} = \mathbf{N}\upsilon^k + (\mathbf{N}_{,x} j_x^k + \mathbf{N}_{,y} j_y^k)/q \qquad (14)$$

$$\mathbf{N} j_x^{k+1} = -qn\mu\mathbf{N}_{,x}\zeta^k + qD_n\mathbf{N}_{,x}\upsilon^k \qquad (15)$$

$$\mathbf{N} j_y^{k+1} = -qn\mu\mathbf{N}_{,y}\zeta^k + qD_n\mathbf{N}_{,y}\upsilon^k \qquad (16)$$

$$[\mathbf{N}_{,xx} + \mathbf{N}_{,yy}]\zeta^{k+1} = -q(N_d - \mathbf{N}\upsilon^k)/\varepsilon \qquad (17)$$

The computations of unknowns are simple and straightforward operations from (14)-(17). Furthermore, if the same collocation points and a constant time-stepping scheme are used throughout the computational process, $\mathbf{N}^{-1}$ computed only once, hence computing υ^{k+1} from υ^k, j^{k+1} from j^k and ζ^{k+1} from ζ^k is a simple operation of $O(N)$.

Similarly as in finite differences, Equation (14) is conditionally stable. However, the stability of the scheme can easily be preserved by an automatic and progressively discarded time sub-divisions as suggested in [8].

IV. Simulation Results

Several choices are possible as radial basis $\phi(\mathbf{x}, \mathbf{x}_i)$, e.g. multiquadratics or spline functions. In this paper, the compactly supported RBF proposed by Wu [9] is used as the radial basis function, $\phi(\mathbf{x}, \mathbf{x}_i)$,

$$\phi(r_i) = \begin{cases} (1 - r_i)^4 (4 + 16r_i + 12r_i^2 + 3r_i^3) & r_i \le 1 \\ 0 & \text{others} \end{cases} \qquad (18)$$

where $r_i = \|\mathbf{x} - \mathbf{x}_i\| / d_{mi}$. Here, d_{mi} represents the supported domain radius at the collocation nodes $\mathbf{x}_i$,

$$d_{mi} = d_{\max} C_i \qquad (19)$$

where $d_{\max}$ is a scaling parameter and C_i at a particular node is determined by searching for enough neighbor nodes such that **A** is non singular everywhere in the domain.

The use of a compactly supported version of the RBF kernel could result in a sparse matrix, and thus decrease the computational cost and memory requirements [10].

The transistor considered in this simulation is a $0.6\,\mu m$ gate MESFET. Fig. 1 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).

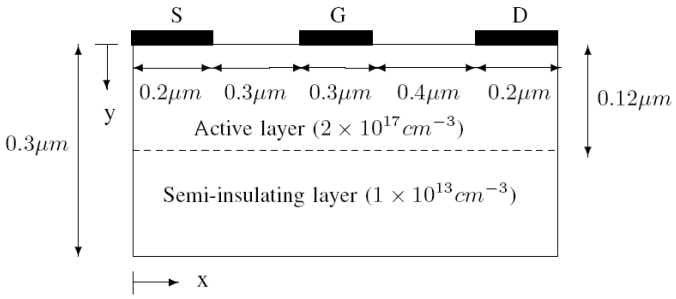

Fig. 1. Cross section of the simulated MESFET.

Since the nodes are uniformly spaced, the value of C_i is set to the distance between two adjacent nodes.

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 potential distribution obtained using the proposed algorithm, while, Fig. 3 illustrates the carrier density distributions. It is significant to indicate that the proposed algorithm gives precisely the same results obtained when the FDTD method is used. The comparison results between the algorithms are not provided because their results coincide exactly on each other when using same points.

After calculating the distributions of potential and carrier density, we can determine where quantities vary rapidly and slowly. In domains that the variation of parameters is high, node generator subprogram add more nodes to initial uniform mesh. By this method, we can generate a nonuniform mesh that is dense in momentous places. Because the dc solution is used in **ac** analysis as initial values and also the level of ac excitation is lower than dc level at most times, therefore one can conclude after applying ac excitation to the structure, the distributions of parameters will fix approximately. For this reason, we can use the nonunifom mesh generated from dc solution in ac analysis.

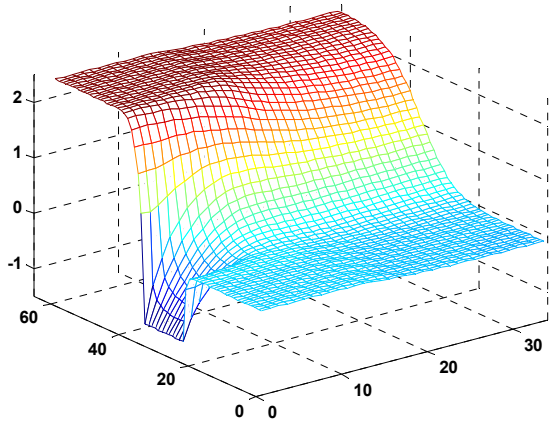

Fig. 2. Potential distribution

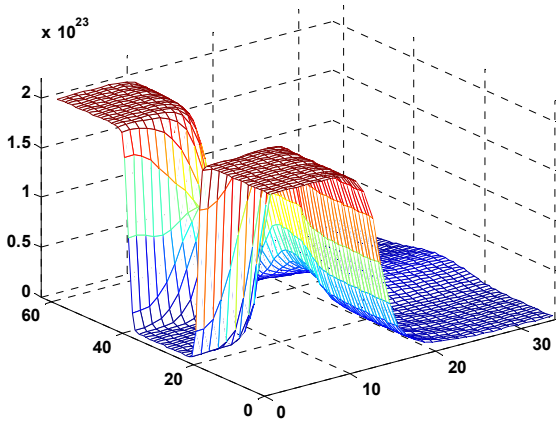

Fig. 3. Carrier density distribution.

VI. Conclusion

This work proposed a numerical method for simulation of time dependent drift-diffusion model of semiconductor devices in two dimensions. The method is remarkably simple, especially for complicated domains and higher dimensions.

Between radial basis functions a compactly supported version has been chosen due to the fact that it can result in a sparse matrix, and thus decrease the computational cost and memory requirements.

Possible extensions of this research are to consider random data nodes and add overlapping domain decomposition method to presented simulation to reduced the computational time.

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