An Efficient Spectral Element Method for Semiconductor Transient Simulation

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Abstract ─ An efficient spectral element method (SEM) based on Gauss-Lobatto-Legendre (GLL) polynomials is proposed for the semiconductor transient simulation. The fully coupled Newton iteration method is employed to solve the nonlinear drift-diffusion model. The mix-order basis functions with different variables and domains are employed to give a full play to the superiority of the proposed SEM. The PIN diode with quasi one-dimensional structure has been analyzed, and the numerical results have demonstrated the efficiency and accuracy of the proposed method.

Index Terms ─ Gauss-Lobatto-Legendre (GLL) polynomials, mix-order basis function, PIN diode, Spectral Element Method (SEM).

I. INTRODUCTION

The drift-diffusion model is a common way to describe the interior carrier behavior of semiconductor devices, and it is a directly-coupled system of three nonlinear partial differential equations [1]. During the past few decades, numerical methods such as finite element method (FEM) and finite difference method (FDM) have been employed to solve the equations [1, 2]. In consideration of the efficiency and accuracy, several adaptive grid refinement strategies have been proposed [3, 4], but the implementation is relatively cumbersome. Recently, the spectral element method (SEM) has shown its higher accuracy and lower computation cost than FEM or FDM [5, 6, 10, 11]. The efficient SEM has been proposed to solve the Schrödinger's equation in nanodevice simulation [7] and the high power microwave propagation problems [8].

In this paper, the spectral element method based on the drift-diffusion model has been developed for semiconductor transient simulation. The Gauss-Lobatto-Legendre (GLL) polynomials are used as the basis function to expand the variables, and it gets the advantage that the error decreases exponentially with the polynomial order increases, called spectral accuracy [8]. To minimize the unknowns, different orders of the basis function can be selected with the following criterion: the higher order of the basis function for the variables with larger range of values such as electron concentration and hole concentration, and the higher order of the basis function for the domain with rapid changing values for the same variable.

The organizations of this article are as follows. In Section II, the basic theory of SEM based on GLL polynomials has been described briefly. Then, the detailed process about how to solve the drift-diffusion model with the spectral element method, and the two strategies that the different orders of the basis function are selected according to the different variables and domains has been introduced specifically. Next, in Section III, the overshoot phenomena in PIN diode with quasi one-dimensional structure has been analyzed to demonstrate the efficiency and accuracy with the proposed method.

II. FORMULATION

The drift-diffusion model is composed of three nonlinear differential equations, the electronic and hole current continuity equations and Poisson equation [2], described as:

$$\begin{aligned} \frac{\partial n}{\partial t} &= \frac{1}{q}\nabla\cdot\mathbf{J}_n + G - R \\ \frac{\partial p}{\partial t} &= -\frac{1}{q}\nabla\cdot\mathbf{J}_p + G - R \\ \nabla^2\varphi &= -\frac{q}{\varepsilon}(N_0 + p - n) \end{aligned}, \tag{1}$$

where φ is the electrostatic potential, q is the electric charge, N_0 is the electrically active net impurity

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concentration, ε is the permittivity, and n and p are the electron and hole carrier densities. G and R describe the generation phenomena and recombination processes. The electron and hole current densities symbolized by $\mathbf{J}_n$ and $\mathbf{J}_p$ are given by:

$$\begin{aligned}\mathbf{J}_n &= qD_n\nabla n - q\mu_n n\nabla\varphi \\ \mathbf{J}_p &= -qD_p\nabla p - q\mu_p p\nabla\varphi,\end{aligned} \tag{2}$$

where D_n and D_p are the corresponding diffusion coefficients, and μ_n and μ_p are the electron and hole mobility.

A. Basis functions

The difference between SEM and FEM lies in the choice of the expansion basis. In order to achieve the high accuracy, the GLL basis functions are employed throughout this article. A rough introduction is shown as follows, and more details can be found in the reference [7].

The Nth order GLL basis functions in a 3-D cubic element $(\xi,\eta,\zeta)\in[-1,1]\times[-1,1]\times[-1,1]$ can be written as:

$$\Phi_{rst}(\xi,\eta,\zeta)=\phi_r^{(N_\xi)}(\xi)\phi_s^{(N_\eta)}(\eta)\phi_t^{(N_\zeta)}(\zeta), \tag{3}$$

for $r=0,1,...,N_\xi; s=0,1,...,N_\eta; t=0,1,...,N_\zeta$. Here, $\phi_r^{(N_\xi)}(\xi)$, $\phi_s^{(N_\eta)}(\eta)$ and $\phi_t^{(N_\zeta)}(\zeta)$ represent the basis functions with three directions and have the following definition:

$$\phi_j^{(\mathrm{N})}=\frac{-1}{N(\mathrm{N}+1)\mathrm{L}_N(\xi_j)}\frac{(1-\xi^2)\mathrm{L}_N'(\xi)}{(\xi-\xi_j)}, \tag{4}$$

Here, $\mathrm{L}_N(\xi)$ and $\mathrm{L}_N'(\xi)$ are the Legendre polynomial of Nth order and its derivative. The points $\{\xi_j, \mathrm{j}=0,1,...,\mathrm{N}\}$ are the zeros of $(1-\xi^2)\mathrm{L}_N'(\xi_j)=0$.

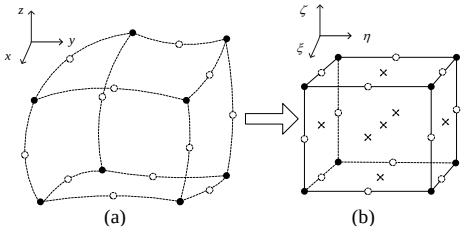

Fig. 1. The mapping from the: (a) physical to the (b) reference domain.

Because of the basis functions definition on the standard cubic element, the mapping from the physical to the reference domain is essential for general meshes as shown in Fig. 1. The basis functions below the physical coordinate and reference one have the following relationship:

$$\begin{cases}N_i=\Phi_i \\ \nabla N_i=\mathbf{J}^{-1}\nabla\Phi_i\end{cases}, \tag{5}$$

where N_i and Φ_i represent the basis functions for the physical and reference coordinate, and $\mathbf{J}$ is the Jacobian matrix.

B. SEM for semiconductor simulation

Here, the electron and hole concentrations and electric potential are selected as the unknown variables. The fully coupled Newton iteration method is employed to solve the nonlinear equations.

Taking electronic current continuity equation for an example, the specific derivation process is introduced here. Firstly, the equation should be normalized into dimensionless form and the factors can be found in [2]. For the time partial derivative, the backward difference operator is employed to achieve the unconditional stability with a large time step represented by Δt:

$$\frac{n^{\mathrm{m}}-n^{m-1}}{\Delta t}=f_n(n^m,p^m,\varphi^m), \tag{6}$$

where $f_n(n,p,\varphi)=\nabla\cdot(\mu_n\nabla n-\mu_n n\nabla\varphi)-(R-G)$, and n^{m} represents the electron carrier densities at the time of $m\Delta t$. The Equation (6) is equivalent to the following form:

$$F_n(n^m,p^m,\varphi^m)=f_n(n^m,p^m,\varphi^m)\cdot\Delta t-\left(n^m-n^{m-1}\right)=0. \tag{7}$$

Expand the formula (7) using the Taylor series and just retain the first order item. Then, the Newton iterative formula can be obtained finally:

$$\begin{aligned}&F_n\left(n^{m,l},p^{m,l},\varphi^{m,l}\right)+\left.\frac{\partial F_n(n,p,\varphi)}{\partial n}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(n^{m,l+1}-n^{m,l}\right)+\\ &\left.\frac{\partial F_n(n,p,\varphi)}{\partial p}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(p^{m,l+1}-p^{m,l}\right)+\left.\frac{\partial F_n(n,p,\varphi)}{\partial\varphi}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(\varphi^{m,l+1}-\varphi^{m,l}\right)=0.\end{aligned} \tag{8}$$

Here, the (n^l,p^l,φ^l) represents the results obtained by the l th Newton iteration. By applying the Galerkin weighted-residual method to (8), the following form (9) can be obtained:

$$\begin{aligned}&\oint_V N_i\cdot F_n\left(n^{m,l},p^{m,l},\varphi^{m,l}\right)dv+\\ &\oint_V N_i\cdot\left.\frac{\partial F_n(n,p,\varphi)}{\partial n}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(n^{m,l+1}-n^{m,l}\right)dv+\\ &\oint_V N_i\cdot\left.\frac{\partial F_n(n,p,\varphi)}{\partial p}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(p^{m,l+1}-p^{m,l}\right)dv+\\ &\oint_V N_i\cdot\left.\frac{\partial F_n(n,p,\varphi)}{\partial\varphi}\right|_{\substack{n=n^{m,l}\\p=p^{m,l}\\\varphi=\varphi^{m,l}}}\left(\varphi^{m,l+1}-\varphi^{m,l}\right)dv=0\end{aligned}. \tag{9}$$

Using the GLL basis functions, the variables can be

expanded as follows:

$$n=\sum_{j=1}^{N_{total}} n_j N_j,\ \ p=\sum_{j=1}^{N_{total}} p_j N_j,\ \varphi=\sum_{j=1}^{N_{total}} \varphi_j N_j, \quad (10)$$

where $N_{total}=(N_\xi+1)(N_\eta+1)(N_\varsigma+1)$ represents the total number of basis functions. Substituting (10) into (9) and simplifying the resulting equation, we have the final form of equation system (11):

$$[\mathbf{EN}]\boldsymbol{\delta}_n^{m,l+1}+[\mathbf{EP}]\boldsymbol{\delta}_p^{m,l+1}+[\mathbf{EF}]\boldsymbol{\delta}_\varphi^{m,l+1}=\mathbf{BE}, \quad (11)$$

where $\mathbf{EN}$, $\mathbf{EP}$ and $\mathbf{EF}$ are the matrices, $\mathbf{BE}$ is the vector, and $\boldsymbol{\delta}_n^{m,l+1}$, $\boldsymbol{\delta}_p^{m,l+1}$ and $\boldsymbol{\delta}_\varphi^{m,l+1}$ are differences between the two values of variables obtained by the l+1th and l th Newton iteration at the time of $m\Delta t$. The elemental matrices are defined as:

$$[\mathbf{EN}]_{ij}=-\Delta t\int\nabla N_i\cdot(-\mu_n(\nabla\varphi^{m,l}\cdot N_j-\nabla N_j))dV - \Delta t\int N_i\cdot N_j\frac{\partial(R-G)^{m,l}}{\partial n}dV-\int N_i\cdot N_j dV, \quad (12)$$

$$[\mathbf{EP}]_{ij}=-\Delta t\int N_i\cdot N_j\frac{\partial(R-G)^{m,l}}{\partial p}dV, \quad (13)$$

$$[\mathbf{EF}]_{ij}=\Delta t\int\mu_n n^{m,l}\nabla N_i\cdot\nabla N_j dV, \quad (14)$$

$$[\mathbf{BE}]_i=\Delta t\int\nabla N_i\cdot(-\mu_n(\nabla\varphi^{m,l}\cdot n^{m,l}-\nabla n^{m,l}))dV+ \Delta t\int N_i\cdot(R-G)^{m,l}dV+\int N_i\cdot(n^{m,l}-n^{m-1})dV. \quad (15)$$

Repeat the above operations for the hole current continuity equation and Poisson equation, then the fully-coupled system can be described by the following matrix form:

$$\begin{pmatrix}\mathbf{EN}&\mathbf{EP}&\mathbf{EF}\\ \mathbf{HN}&\mathbf{HP}&\mathbf{HF}\\ \mathbf{PN}&\mathbf{PP}&\mathbf{PF}\end{pmatrix}\begin{pmatrix}\boldsymbol{\delta}_n^{m,l+1}\\ \boldsymbol{\delta}_p^{m,l+1}\\ \boldsymbol{\delta}_\varphi^{m,l+1}\end{pmatrix}=\begin{pmatrix}\mathbf{BE}\\ \mathbf{BH}\\ \mathbf{BP}\end{pmatrix}. \quad (16)$$

The remaining elemental matrices are defined as:

$$[\mathbf{HN}]_{ij}=-\Delta t\int N_i\cdot N_j\frac{\partial(R-G)^{m,l}}{\partial n}dV, \quad (17)$$

$$[\mathbf{HP}]_{ij}=\Delta t\int\nabla N_i\cdot(-\mu_p(\nabla\varphi^{m,l}\cdot N_j+\nabla N_j))dV- \Delta t\int N_i\cdot N_j\frac{\partial(R-G)^{m,l}}{\partial p}dV-\int N_i\cdot N_j dV, \quad (18)$$

$$[\mathbf{HF}]_{ij}=-\Delta t\int\mu_p p^{m,l}\nabla N_i\cdot\nabla N_j dV, \quad (19)$$

$$[\mathbf{BH}]_i=-\Delta t\int\nabla N_i\cdot(-\mu_p(\nabla\varphi^{m,l}\cdot p^{m,l}+\nabla p^{m,l}))dV+ \Delta t\int N_i\cdot(R-G)^{m,l}dV+\int N_i\cdot(p^{m,l}-p^{m-1})dV, \quad (20)$$

$$[\mathbf{PN}]_{ij}=\int N_i\cdot N_j dV, \quad (21)$$

$$[\mathbf{PP}]_{ij}=\int N_i\cdot N_j dV, \quad (22)$$

$$[\mathbf{PF}]_{ij}=\int\nabla N_i\cdot\nabla N_j dV, \quad (23)$$

$$[\mathbf{BP}]_i=-\int\nabla N_i\cdot\nabla\varphi^{m,l}dV-\int N_i\cdot(n^{m,l}-p^{m,l}-N_0)dV. \quad (24)$$

When the norm of $(\boldsymbol{\delta}_n^{m,l+1},\boldsymbol{\delta}_p^{m,l+1},\boldsymbol{\delta}_\varphi^{m,l+1})^T$ is less than the setting of tolerance, $(\mathbf{n}^{m,l+1},\mathbf{p}^{m,l+1},\boldsymbol{\varphi}^{m,l+1})^T$ can be account as the approximate solution of the original nonlinear system.

Particularly, it may suffer from instability when a simple finite difference scheme is employed as mentioned in [12]. The numerical error is caused by the hyperbolic and convection dominated equations. The stability of the model can be improved by employing proper discretization method. In this paper, the backward Euler scheme in time and GLL basis functions in space are employed. The backward Euler scheme is implicit and unconditionally stable with large time steps. As a specific finite element method, the SEM with GLL basis functions also satisfies the discrete maximum principle [13]. Therefore, the proposed method can yield a reasonable degree of accuracy independent of perturbations.

C. Mix-order basis function

Here, the electron and hole concentrations and electric potential are selected as the unknown variables. The fully coupled Newton iteration method is employed to solve the nonlinear equations. The variation range of the electron and hole carrier densities is still larger than electrostatic potential by expressing all densities in units of n_i and all potential in units of kT/q, where n_i is the intrinsic density, k is the Boltzmann's constant and T is the carrier temperature [2]. To capture the density gradient, the fine meshes or the higher order basis function is necessary. Based on the above consideration, different orders of the basis function can be selected by the range and the changing domain of the three variables. Here, we employ higher order for the electron and hole carrier densities and higher order for the rapid changing domain with the same variable. Because of using different orders of basis function for carrier densities and potential, the following integration is needed to fill the above matrices, taking the $[\mathbf{T}]_{ij}$ for example:

$$\begin{aligned}&\int_{\Omega_e}N_iN_jdV\\ &=\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\Phi_i\Phi_j|\mathbf{J}|d\xi d\eta d\zeta\\ &=\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1}\phi_m^{(N_\xi)}(\xi)\phi_n^{(N_\eta)}(\eta)\phi_p^{(N_\varsigma)}(\zeta)\cdot\phi_{m'}^{(N'_\xi)}(\xi)\phi_{n'}^{(N'_\eta)}(\eta)\phi_{p'}^{(N'_\varsigma)}(\zeta)|\mathbf{J}|d\xi d\eta d\zeta\\ &=\sum_{r=0}^{N_\xi}\sum_{s=0}^{N_\eta}\sum_{t=0}^{N_\varsigma}|J_{rst}|w_rw_sw_t\phi_m^{(N_\xi)}(\xi_r)\phi_n^{(N_\eta)}(\eta_s)\phi_p^{(N_\varsigma)}(\zeta_t)\cdot\phi_{m'}^{(N'_\xi)}(\xi_r)\phi_{n'}^{(N'_\eta)}(\eta_s)\phi_{p'}^{(N'_\varsigma)}(\zeta_t),\end{aligned} \quad (25)$$

N_i and N_j have different orders and the high order integration is employed with $(N_\xi>N'_\xi, N_\eta>N'_\eta, N_\varsigma>N'_\varsigma)$.

Due to the fact that different domain has different order of basis functions, the continuity at the interface between two domains must be handled properly. Considering that the quasi one-dimensional structure is analyzed in this paper, the different orders basis functions are only applied at the direction with changing variables. Therefore, the continuity can be enforced easily.

III. NUMERICAL EXAMPLES AND DISCUSSIONS

In order to verify the accuracy and efficiency of the proposed method, the quasi one-dimensional PIN diode with the p^+nn^+ doping is selected as the numerical model [9]. As shown in Fig. 2, the cross section area of the diode is $10^{-8}cm^2$, and the length is 10 μm. The distribution of doping concentration is displayed by Fig. 3.

Here, it should be indicated that all the numerical examples are computed on an Intel(R) Core(TM)2 with 2.83 GHz CPU (the results are computed by only one processor) and 8 GB RAM. The tolerance is set to be 10^{-6}.

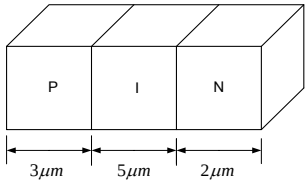

Fig. 2. The model of PIN diode.

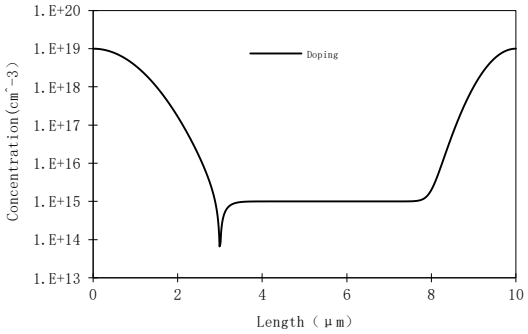

Fig. 3. The doping concentration of PIN diode.

A. Basic simulation

In order to verify the validity of the proposed SEM for transient semiconductor simulation, a sine-wave voltage is imposed on the anode of the PIN diode. The mesh size is 0.01 μm, and the order of the basis functions is set to be 1. The time step size is 1 *ns*. Figure 4 shows the transient current flowing through the diode, and it is in good agreement with the result obtained by COMSOL software.

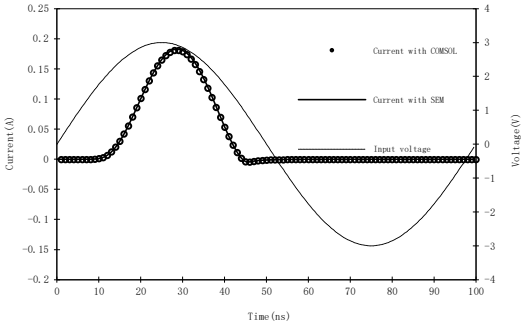

Fig. 4. The distribution of transient current.

Figure 5 shows the distribution of variables at the time of 20 *ns*, and the results of the comparison with COMSOL demonstrate the validity of the SEM for transient semiconductor simulation.

B. Mix-order with variables and domains

It can be found that the electron and hole carrier densities have a faster change than the electric potential from Fig. 5. Therefore, it is reasonable to use high order basis function for densities and low one for potential. As can be seen in Fig. 5, the densities in P domain and N domain have larger gradient than I domain. So, the high order basis functions are employed for the variables in P domain and N domain.

To verify the efficiency of the mix-order basis function with different variables and domains, the transient response under the electromagnetic pulse with fast rise time has been simulated. Figure 6 shows the input voltage imposed on the anode of the diode, and gives the transient current densities obtained by SEM with 1st order and 5th order basis function. The mesh size for 1st order basis function is 0.01 μm and 0.2 μm for 5th order basis function. The time step size is 1 ps. The overshoot current shown in Fig. 6 is due to the capacitive performance of PIN diode under high frequency.

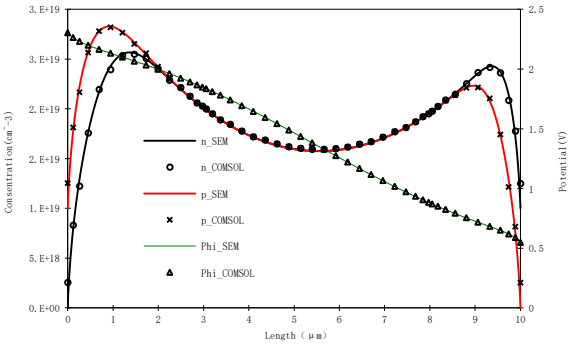

Fig. 5. The distribution of variables at the time of 20 ns.

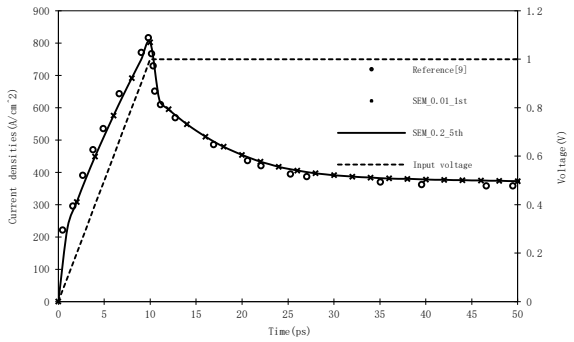

Fig. 6. The distribution of transient current densities.

Table 1 shows the compute time using the mix-order basis functions with different variables. The same high order basis functions for the electron and hole carrier densities, and low order basis functions for electric potential. Table 2 shows the compute time using the mix-order basis functions with different variables and different domains. The same high order basis functions for the P and N domain, and low order basis functions for I domain. As can be seen in Table 2, the case with standard 1st order of basis function takes 3.32 times CPU time than the proposed mix-order method. The proposed mix-order SEM exhibits a good efficiency in semiconductor transient simulation.

Table 1: Comparison of computation Efficiency

Mesh Size (μm)	Order of Basis Function		Number of Unknowns	CPU Time (s)
	n, *p*	φ		
0.01	1st	1st	11988	206
0.1	4th	4th	4788	177
	4th	1st	3588	132
0.2	5th	5th	2988	148
	5th	2nd	2388	112

Table 2: Comparison of computation efficiency

Mesh Size (μm)	Order of Basis Function		Number of Unknowns	CPU Time (s)
	n, *p*	φ		
0.01	1st	1st	11988	206
0.1	4th	1st	3588	132
	4th (2nd)	1st	2788	88
0.2	5th	2nd	2388	112
	5th (2nd)	2nd (1st)	1688	62

The numbers in the bracket represent the orders of basis functions for I domain. The default represents the same order of basis function for the whole domain.

VI. CONCLUSION

In this paper, the spectral element method (SEM) is proposed for the semiconductor transient simulation. The Gauss-Lobatto-Legendre (GLL) polynomials are used as the basis function to expand the variables. The fully coupled Newton iteration method is employed to solve the nonlinear drift-diffusion model. The mix-order basis functions with different variables and domains are employed to improve the compute efficiency. The PIN diode with quasi one-dimensional structure has been analyzed, and the numerical results demonstrate the accuracy and efficiency with the proposed method.

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