Numerical Solution of Hydrodynamic Semiconductor Device Equations Employing a Stabilized Adaptive Computational Technique

YIMING LI[*] and CHUAN-SHENG WANG[a]
National Nano Device Laboratories, and
Microelectronics and Information Systems Research Center
National Chiao Tung University
[a]Department of Mathematics, National Tsing Hua University
[*]Corresponding address: 1001 Ta-Hsueh Rd., Hsinchu city, Hsinchu 300
TAIWAN

Abstract: - In this paper, we generalize our proposed earlier computing method [10-11] to solve hydrodynamic semiconductor device equations. For submicron MOSFET devices, we simulate their temperature distribution by solving carrier energy balance equation with adaptive computational technique. This robust method based on: (1) the finite volume (FV) discertization scheme; (2) the monotone iterative (MI) algorithm; (3) a posteriori error estimation; and (4) the 1-irregular mesh refinement; is successfully developed and implemented. Numerical results not only have a good agreement with physical phenomena but also demonstrate that our methodology has good computational efficiency. Convergence property for arbitrary initial guesses for the beginning of simulation is also reported to show the robustness of the method.

Key-Words: - Hydrodynamic Equations, Semiconductor Device Simulation, MOSFET, Adaptive Computation, Error estimation, Monotone Iterative Technique, Carrier Temperature

1. Introduction

For microelectronics, the progress of semiconductor fabrication technology for the advanced metal oxide semiconductor field effect transistor (MOSFET) has been of great interests [1-2] in recent years. The device channel lengths are so small that nonlocal effects and source/drain engineering become more important for the device characteristics and performance. Despite significant advances over the last decade, TCAD (technology computer-aided design) must progress even more dramatically during the 2000s if simulation is to live up the high expectations of the user community. The TCAD approach [2] provides a direct alternative to study the intrinsic and extrinsic electrical behavior for these MOSFET structures at a very fundamental physical level. In recent years, especially for the ultra-small MOSFET device, it has become a very important tool in the development of new devices and fabrication technologies [2-15]. The aim of our works is to develop an efficient and intelligent physical-based TCAD tools for the day-to-day micron and nano advance CMOS design.

To study the effects mentioned above for ultra-short channel MOSFET devices, an energy balance equation should be solved numerically for carrier temperature distribution [10-13]. Simulated results can be applied for the further optimal design and characterization.

To study the variation of carriers temperature and their physical mechanism inside a submicron MOSFET device, a hydrodynamic model including at least the energy balance equation in a device simulation should be solved, and this approach has been received many notices. Various simulation approaches have been proposed for the numerical solution of this equation efficiently [3-15]. The rapid variation of electron temperature within very small regions leads to a significant difficulty in semiconductor device simulation. This electron temperature model problem is so-called a singular nonlinear boundary value problem. It has the numerical stability and the convergence problems when solving the system of nonlinear algebraic equations arising from the discretization of such energy balance equation. The well known Scharfetter-Gummel-Tang (SGT) scheme [13-15] for solving this problem holds only for very fine mesh artificially. However, it goes without saying that the arrangement of the fine mesh to fit the SGT assumption is surely a difficult task.

In this paper, we further generalize our proposed earlier computing algorithm for the intelligent

numerical solution of semiconductor device energy balance equation using not only monotone iterative algorithm but also adaptive mesh refinement rule. First of all, we solve a set of drift diffusion (DD) equations with our developed device simulator earlier [3-9]. The computed physical quantities, such as electron concentration, electrostatic potential, and electron current are used as the input data for carrier temperature simulation. According to our methodology [3-11], the energy balance equation is transformed into another partial differential equation (PDE) with having a self-adjoint form and then discretized using adaptive finite volume method with 1-irregular unstructured mesh. The adaptive FV discretized energy balance equation leads to a system of nonlinear algebraic equations with a diagonal dominate property. We solve the nonlinear system by applying a monotone iterative method directly. With the developed carrier temperature simulator, we study basic physical energy variation mechanism for a submicron NMOSFET under high bias condition. The numerical results and convergence property of the algorithm are also reported in this work.

This paper is organized as follows. In Sec. 2, we briefly state energy balance equations associated physical models. In Sec. 3, we present the overall adaptive computational procedure for the carrier temperature calculation. In Sec. 4, simulation results for a submicron N-MOSFET device are presented to demonstrate the robustness and efficiency of the method. Sec. 5 draws the conclusion and suggests the future work.

2. A Hydrodynamic Model

We state a hydrodynamic (HD) model that includes a drift diffusion (DD) model and energy balance equations for electrons and holes. The DD model was derived from the Maxwell's equation as well as charge conservation law.

$$\Delta f = \frac{q}{e_S}(n - p + D), \tag{1}$$

$$\frac{1}{q}\nabla \cdot \mathbf{J}_n = R(n, p), \tag{2}$$

$$\frac{1}{q}\nabla \cdot \mathbf{J}_p = -R(n, p), \tag{3}$$

$$\mathbf{J}_n = -qm_n n\nabla f + qD_n \nabla n, \tag{4}$$

$$\mathbf{J}_p = -qm_p p\nabla f - qD_p \nabla p. \tag{5}$$

Eq. (1) is so-called the Poisson equation. The Eqs. (2) and (3) derived from the charge conservation law are the electron and hole continuity equations. The Eqs. (4) and (5) are electrons and holes current equations, respectively. The unknown $f = f(x,y)$ to be solved is the electrostatic potential; n and p are electrons and holes concentrations. The function $D = -(N_D^+ - N_A^-)$, in Eq. (1), is the specified ionized net doping profile, and $R = R(n,p)$ is the recombination rate for electrons and holes [1]. The quantity $q = 1.60218 \times 10^{-19} C$ is the elementary charge; $e_S = 11.9 e_0$ is silicon permittivity. The N_D^+, and N_A^- are ionized donor and acceptor impurities, and $e_0 = 8.85418 \times 10^{-14} F/cm$ is the permittivity in vacuum. The D_n, D_p, μ_n, and μ_p are electron and hole diffusion coefficients and mobility functions, respectively [1]. This DD model contains Eqs. (1) – (5), and was solved successfully in our earlier works [3-9].

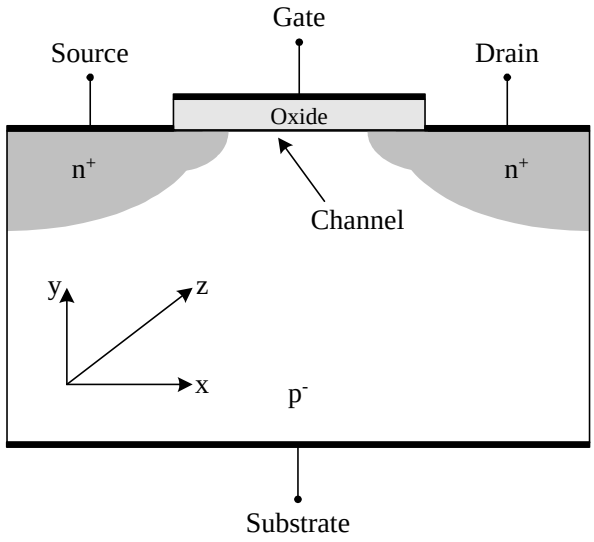

Fig. 1. A two-dimensional cross section domain for a submicron N-MOSFET device.

The HD model contains energy balance equations for electrons and holes. It will be solved for studying the carrier temperature variation.

$$\nabla \cdot \mathbf{S}_n = \mathbf{J}_n \cdot \mathbf{E} - \frac{n(w_n - w_0)}{t_{nw}(T_n)}, \tag{6}$$

$$\nabla \cdot \mathbf{S}_p = \mathbf{J}_p \cdot \mathbf{E} - \frac{p(w_p - w_0)}{t_{pw}(T_p)}. \tag{7}$$

$$\mathbf{S}_n = \frac{\mathbf{J}_n}{-q} w_n + \frac{\mathbf{J}_n}{-q} k_B T_n + \mathbf{Q}_n, \tag{8}$$

$$\mathbf{S}_p = \frac{\mathbf{J}_p}{-q} w_p + \frac{\mathbf{J}_p}{+q} k_B T_p + \mathbf{Q}_p, \tag{9}$$

where the notations as well as the physical models are followed our conventional symbols and can be found in [10-11]. In Sec. 3, we apply the adaptive FV and MI methods to solve the above HD equations. With those computed physical quantities from the DD equations, the energy balance equations are then solved to obtain the carrier temperature distribution over the device structure.

As shown in Fig. 1, the HD equations (1)-(9) are subject to mixed type boundary conditions in a two-dimensional simulation domain. On the left and right sides, the homogeneous Neumann type boundary condition is considered. On the Source, Gate, Drain and Substrate contacts, the Dirichlet type boundary condition is applied [1,3-15]. The proposed adaptive solution procedure for the numerical solution of these equations will be discussed in Sec. 3.

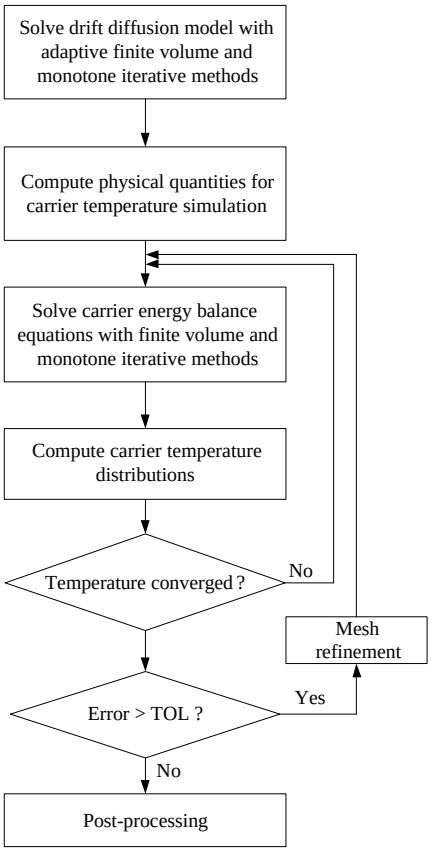

Fig. 2. An overall simulation procedure for a HD semiconductor device simulation.

3. Adaptive Simulation Technique

As shown in Fig. 2, with the computed results from the DD model in advanced, we solve energy balance equations (6)-(9), subsequently. To calculated electrostatic potential, electric field, carrier concentrations, and current flows, Eqs. (1)-(5), the drift diffusion equations are solved with the Gummel's decoupled algorithm [3-9,14-15] and monotone iterative method [3-9]. Here we briefly state the flowchart and numerical methods for the solutions of drift diffusion model which can be found in our earlier works [3-9]. The well-known Gummel's decoupled method is that the device equations are solved sequentially For the numerical solution of semiconductor device DD model, the Poisson's equation is solved for $f^{(g+1)}$ given the previous states $u^{(g)}$ and $v^{(g)}$. The electron current continuity equation is solved for $u^{(g+1)}$ given $f^{(g)}$ and $v^{(g)}$. The hole current continuity equation is solved for $v^{(g+1)}$ given $f^{(g)}$ and $u^{(g)}$. The superscript index g denotes the Gummel's iteration loops. Each the decoupled PDE is solved adaptively [3-9]. Decoupled equation is discretized with the FV method. The corresponding nonlinear system is solved with the MI algorithm. When a converged solution is computed, we perform error estimation of the results for all elements. If the solution does not satisfy the specified stopping criterion (TOL), we will run the mesh refinement and repeat the computation. The results obtained from the DD model are used as the input data for the numerical solutions of the carrier balance equations (6)-(9).

The conventional algorithm for the numerical solution of electrons and holes energy balance equation in semiconductor device simulation consists of: (i) applying the FV (or so-called the finite box) method to discretize the equations; (ii) using Scharfetter-Gummel-Tang scheme, an exponential fitting liked algorithm, [10-15] for the electron and hole energy balance equations to construct a system of nonlinear algebraic equations; (iii) solving the nonlinear system with Newton's iteration method; and (iv) repeating the step (iii) until the solution converged. Our simulation algorithm, as shown in Fig. 2, not only replaces Newton's iteration by the MI method but also applies the adaptive computing method [3-9] for a posteriori error estimation and automatic mesh refinement. The system of nonlinear algebraic equations arising from adaptive FV discretization on a 1-irregular unstructured mesh, as shown in Fig. 3, forms to a nonlinear system (10), where the matrix **A** can be proved that it is still a M-matrix.

$$\mathbf{Az} = -\mathbf{F}(\mathbf{z}), \tag{10}$$

where **z** is the unknown vector, **F** is the nonlinear vector form, and **A** is the corresponding matrix, respectively. Based on our previous observations

[10-11] the nonlinear property of the right hand side of the eqations (6)-(9) is the monotone functions in its unknown, we have a similar result concerning the well-posed problem for the adaptively discretized energy balance equations.

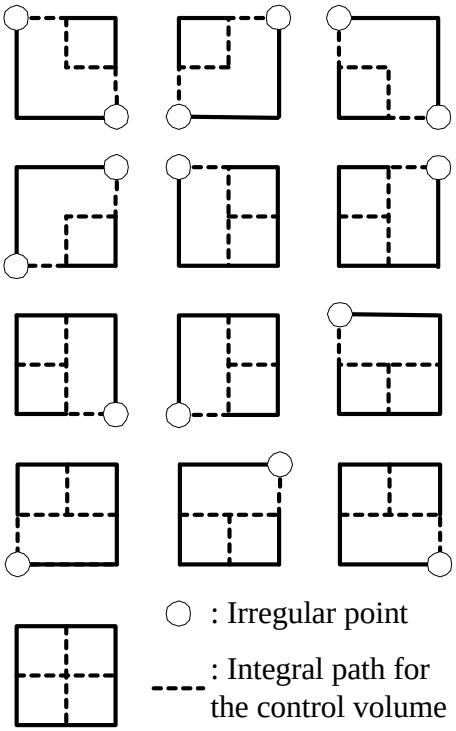

Fig. 3. 13-types 1-irregulr mesh structure.

For a certain type of the 1-irregular mesh structures, as shown in Fig. 4, the nonlinear system in component-wise form and the entries of the matrix **A** is as followed.

$$\begin{aligned} &-x_{i,j-1}z_{i,j-1} - x_{i-1,j}z_{i-1,j} + x_{i,j}z_{i,j} - x_{i+1,j}z_{i+1,j} \\ &-x_{i,j+1}z_{i,j+1} - x_{i+1/2,j+1/2}z_{i+1/2,j+1/2} = -F(z_{i,j}), \end{aligned} \tag{11}$$

In Eq. (8), it can be verified that all coefficients are nonnegative and satisfy the conditions

$$x_{i,j} \geq x_{i+1,j} + x_{i-1,j} + x_{i,j+1} + x_{i,j-1} + x_{i+1/2,j+1/2}, \tag{12}$$

for all discretization index (*i*,*j*) in the device domain. For other cases, we have the similar results and properties; therefore we can prove the following result immediately.

Theorem 1 *The nonlinear system* (10) *arising from above adaptive finite volume discretization scheme has at most a solution.*

Furthermore, the monotone iterative scheme for the corresponding discretized nonlinear system (10) is of the following form [3-11]:

$$(\mathbf{D} + l\mathbf{I})\mathbf{Z}^{(m+1)} = (\mathbf{L} + \mathbf{U})^{(m)} - \mathbf{F}(\mathbf{Z}^{(m)}) + l\mathbf{I}\mathbf{Z}^{(m)}, \tag{13}$$

where **z** is the unknown vector, **F** is the nonlinear vector form, and **D**, **L**, **U**, and **I** are diagonal, lower triangular, upper triangular, and identity matrices, respectively. The monotone iterative parameter l is determined node-by-node depending on the device structure, doping concentration, bias condition, and nonlinear property of each decoupled equation.

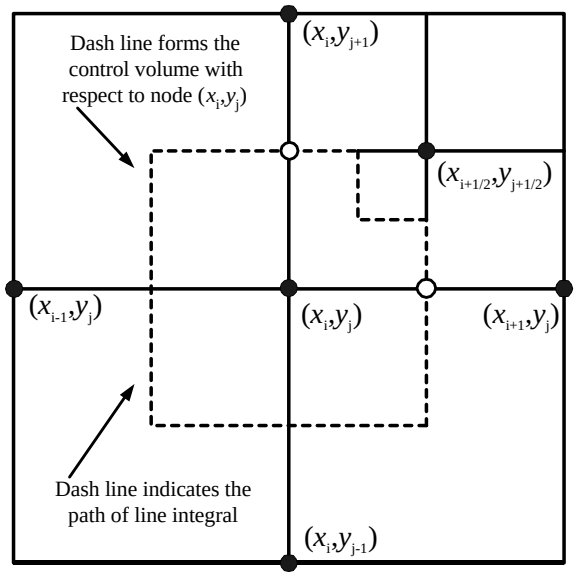

Fig. 4. One of the 13 types of the 1-irregular mesh structure.

The MI method applied here for semiconductor device temperature simulation [3-11] is not only ready for parallelization but also a global method (i.e., it does not require a sufficiently accurate initial guess to begin with the solutions). Once the approximated solutions are computed we do a error estimation and then the mesh refinement following the rule of the 1-irregular unstructured mesh [3-9].

4 Simulation Results and Discussion

In this section, to test the robustness of the method we present here the computed electron temperature distribution for a 0.25 μm N-MOSFET device at high bias condition. Similarly, holes temperature can be calculated with the proposed method. The required electron concentration, electrostatic potential, electric field, and electron current density are computed directly from the DD model in advance. This tested device has a Gaussian distribution doping

profile. The gate oxide thickness equals 7 nm; the ratio of device width and channel W/L_{eff} equals 40/0.25 and V_{BS} = 0V. The profiles have their maximum values $10^{20}/cm^3$ in both the source and drain, where the substrate doping is of $10^{16}/cm^3$.

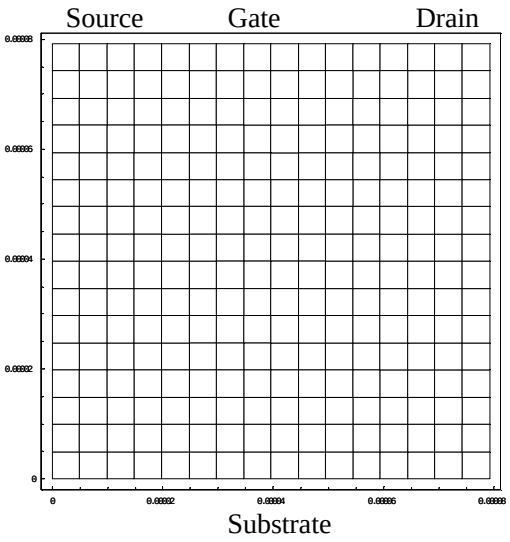

Fig. 5. Initial mesh for the adaptive computation.

Fig. 5 shows the initial mesh applies to simulate the N-MOSFET device temperature distribution. It contains 256 elements. The applied voltage for this device is V_{DS} = V_{GS} = 2.0V, respectively. The Fig. 6 shows a final refined mesh for the numerical solutions of the carrier energy balance equations. In our calculation experience, it takes about 7 refinements to satisfy the specified stopping criterion. This refined mesh contains about 48000 elements in the simulation domain. With the error estimation, the unstructured mesh is generated automatically.

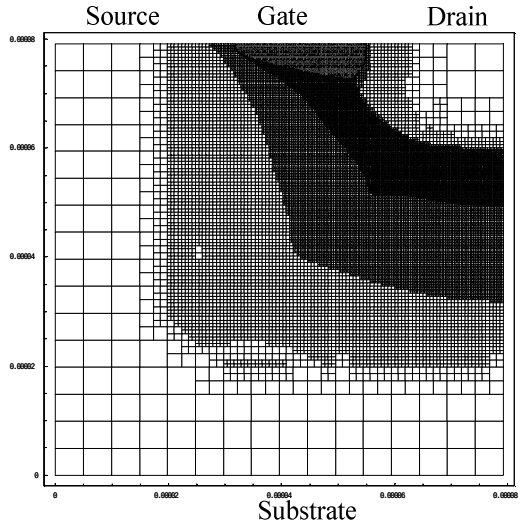

Fig. 6. A refined mesh for the adaptive computation.

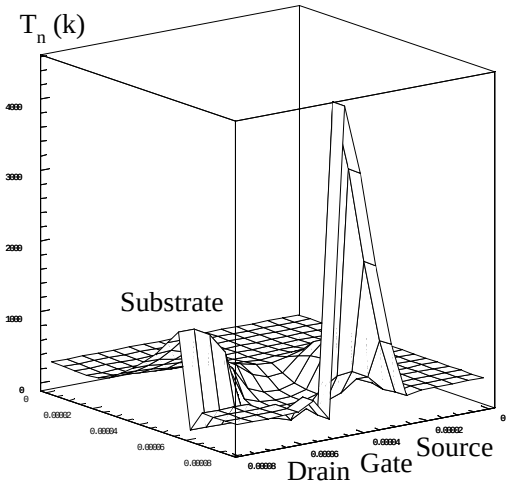

Fig. 7. Computed electron temperature of the N-MOSFET with the initial mesh.

Fig. 7 presents the computed electron temperature with the initial mesh. The result is a rather rough data. After the error estimation and the 1-irregular mesh refinement; we find, as shown in Fig. 8, the result is excellent and has its physical meaning that the temperature attains its maximum near the channel and the drain side. Compared with the conventional structure mesh, our adaptive mesh and solution technique have their robustness and improve the quality of the solution significantly.

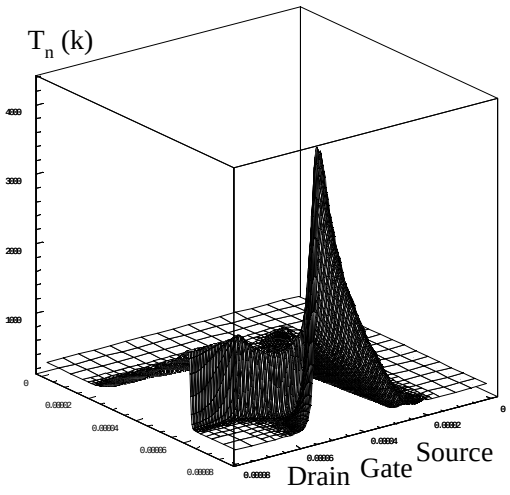

Fig. 8. Electrons temperature with the final refined mesh. This tested 0.25μm N-MOSFET devices is with V_{DS} = V_{GS} =2.0V

With the developed HD simulator, we have calculated the electron temperature for the conventional N-MOSFET structure and it is about 4900 k at V_{DS} = V_{GS} = 2.0V. The high temperature is due to the high electric field at the drain side and can be further improved with the LDD drain engineering [1,10-11]. As shown in Fig. 9, we present the global convergence property of the adaptive FV and MI

algorithms for the numerical solution of energy balance equations. It confirms that the MI method for device simulation has its robustness.

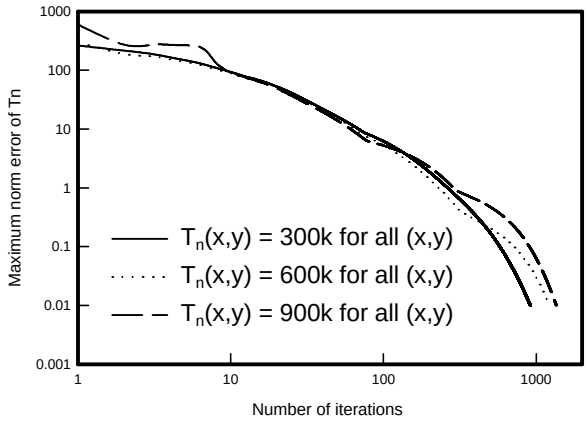

Fig. 9. Convergence behavior for unknown T_n in the monotone iteration loop.

5 Conclusion

In this paper we have successfully generalized our proposed earlier simulation technique to calculate electron temperature by solving a HD model adaptively. This approach relied on the MI method, a posteriori error estimation and 1-irregular mesh refinement technique has been developed and implemented. Numerical results for a submicron N-MOSFET show the robustness and efficiency of the method. In the future work, we plan to extend this adaptive computing method for advanced quantum transport equations simulation.

Acknowledgement

This work was supported in part by the National Science Council of Taiwan under Contract No. NSC 90-2112-M-317-001.

References:

[1] S. M. Sze, *Physics of Semiconductor Devices*, 2nd Ed., Wiley-Interscience, New York, 1981.

[2] R. Dutton, et al., "Perspectives on Technology and Technology - Driven CAD.," *IEEE Trans. CAD*, 19, 2, 2000, pp. 1544-1560.

[3] Y. Li, et al., "*Monotone Iterative Method and Adaptive Finite Volume Method for Parallel Numerical Simulation of Submicron MOSFET Devices*," in "Topics in Applied and Theoretical Mathematics and Computer Science" Ed. by V. V. Kluev, et al., WSEAS Press, Dec. 2001, pp. 25-30.

[4] Y. Li, et al., "A Domain Partition Approach to Parallel Adaptive Simulation of Dynamic Threshold Voltage MOSFET," *Abst. Book Conference on Computational Physics 2001*, Aachen, Sep. 2001, p. O38.

[5] Y. Li, et al., "*Monotone Iterative Method for Parallel Numerical Solution of 3D Semiconductor Poisson Equation*," in "Advances in Scientific Computing, Computational Intelligence and Applications" Ed. by N. Mastorakis, et al., WSES Press, July 2001, pp. 54-59.

[6] Y. Li, et al., "Parallel Dynamic Load Balancing for Semiconductor Device Simulations on a Linux Cluster," *Tech. Proc. 2001 4th Inter. Conf. Modeling and Simulation of Microsystem*, South Carolina, March 2001, pp. 562-566.

[7] Y. Li, "A Monotone Iterative Method for Semiconductor Device Drift Diffusion Equations," *WSEAS TRANSACTIONS ON SYSTEMS*, 1, 1, 2002, pp. 68-73.

[8] Y. Li, et al., "A new parallel adaptive finite volume method for the numerical simulation of semiconductor devices," *Comput. Phys. Comm.*, 142, 1-3, 2001, pp. 285-289.

[9] Y. Li, et al., "A Novel Approach for the Two-Dimensional Simulation of Submicron MOSFET's Using Monotone Iterative Method," IEEE *Proc. Inter. Symp. VLSI-TSA*, Taipei, June 1999, pp. 27-30.

[10] Y. Li, "A Novel Approach to Carrier Temperature Calculation for Semiconductor Device Simulation using Monotone Iterative Method. Part I: Numerical Algorithm," *Proc. 3rd WSEAS Symp. Math. Methods Comput. Tech. Electrical Eng.* (*MMACTEE 2001*), Athens, Dec. 2001, pp. 5671-5676.

[11] Y. Li, "A Novel Approach to Carrier Temperature Calculation for Semiconductor Device Simulation using Monotone Iterative Method. Part II: Numerical Results,"*Proc. 3rd WSEAS Symp. Math. Methods Comput. Tech. Electrical Eng.* (*MMACTEE 2001*), Athens, Dec. 2001, pp. 5721-5726.

[12] K. Blotekjaer, "Transport Equations for Electrons in Two-Valley Semiconductors," *IEEE Trans. Elec. Dev.*, 17, 1970, pp. 38-47.

[13] T.-W. Tang, "Extension of the Scharfetter-Gummel Algorithm to the Energy Balance Equation," *IEEE Trans. Elec. Dev.*, 31, 12, 1984, pp. 1912-1914.

[14] J. W. Jerome, *Analysis of Charge Transport: A Mathematical Study of Semiconductor Devices*, Springer-Verlag, New York, 1996.

[15] M. Ieong, et al., "Influence of Hydrodynamic Models on the Prediction of Submicrometer Device Characteristics," *IEEE Trans. Eelc. Dev.*, 44, pp. 2242-2251, 1997.