Adaptive Monte Carlo Method for the Solution of Semiconductor Poisson-Boltzmann Transport Equations

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Abstract: In this paper we propose a parallel and adaptive 1-irregular mesh simulation technique for the Monte Carlo solution of semiconductor Poisson-Boltzmann transport equations. We iteratively solve the coupled Poisson and Boltzmann transport equations using Monte Carlo particle method on an unstructured mesh for 1D/2D $n^+\!-\!n\!-\!n^+$ device. Most of the conventional particle approaches for simulating semiconductor Poisson-Boltzmann transport model are relied on fine structure mesh, so it is a time-consuming task and has significantly statistical noise. Based on adaptive 1-irregular mesh, monotone iterative method, and a posteriori error estimation method, the proposed simulation is developed and successfully implemented on a 16-PC's Linux-cluster with message passing interface libraries. Monte Carlo simulation on an unstructured 1-irregular mesh has more computational efficiency than the conventional simulation on structured mesh. It can be utilized for large-scale and 2D/3D nanometer scale device simulation. Our primary results including potential, electron density, energy, and velocity for an $n^+\!-\!n\!-\!n^+$ structure are presented to show the novelty and robustness of this method.

Key-Words: Adaptive Mesh Refinement, Monte Carlo Method, Poisson-Boltzmann Transport Equation, Monotone Iterative Method, Cluster Computing, $n^+\!-\!n\!-\!n^+$ device

1 Introduction

Advances in semiconductor fabrication technology have allowed the continual reduction of minimum feature sizes consistent with Moore's Law. Gordon Moore made his famous observation in 1965, just 4 years after the first planar integrated circuit (IC) was discovered. The press called it "Moore's Law" and the name has stuck. In his paper [1], Moore predicted that the number of transistors per IC would double every 18 months. The Semiconductor Industry Association has projected this trend to continue for at least the next 15 years, aggressively pushing the bit count of DRAM by a factor of 4 every 3 years.

Among the grand challenges for high performance computing, nanoscale device physics, simulation, and characterization are of particular interest for their roles in developing a key industrial technology. This continual downsizing of device sizes has placed tremendous demands on predicting the behavior of designs [2,3]. TCAD/ECAD tools [4] for device simulation can considerably reduce the development cost and turnaround time for new devices. However, aggressive scaling of semiconductor technology is pushing the capabilities of today's simulation tools. Carrier transport in commercial TCAD packages is usually described with the drift diffusion or hydrodynamic models. However, these models may not adequate, because they hold only if the carriers are supposed to be in thermal equilibrium with the lattice (which is not the case in the high field and almost ballistic situations encountered in deep-submicron and nanoscale devices). The Monte Carlo Method (MCM) for semiconductor device simulation [5-11], which is based on a microscopic approach of electrons in semiconductors, offers an alternative that is becoming increasingly important as device technology now focuses on the nanometer scale ULSI regime, where device sizes are less than 0.18 μm. From the MCM simulation, a detailed description of the underlying physics of the device behavior can be gleaned. Nevertheless, the large computational requirements of MCM, which may be on the order of hours or days of CPU time even for 2D treatments on high performance systems, prohibit its direct use in practical device engineering. An efficient application of MCM has therefore remained either for research or as a method of parameter extraction for higher-level models.

In this paper, based on our previous works for deep-submicron semiconductor device simulation with adaptive and parallelization methods, we propose an adaptive 1-irregular mesh simulation technique for MCM solution of the Poisson-Boltzmann Transport Equations (P-BTE) on a Linux-cluster. This approach is a direct extension of the parallel adaptive computing method for solving device models in our
earlier works [12-18]. We for the first time iteratively solve the coupled P-BTE model using MCM on an unstructured mesh for 1D/2D $n^+ - n - n^+$ device. Conventional MCMs for solving P-BTE model are with fine structure mesh. They are time-consuming task and have significantly statistical noise. Our adaptive MCM bases on adaptive 1-irregular mesh, monotone iterative, and a posteriori error estimation methods on a Linux-cluster. Our simulation results for an $n^+ - n - n^+$ structure show that perform MCM simulation on an unstructured 1-irregular mesh has more computational efficiency than the conventional simulation on structured mesh. It can be utilized for multidimensional nanomter scale device simulation.

This paper is organized as follows. Sec. 2 states the P-BTE model. Sec. 3 presents the adaptive solution scheme, iterative method, and the parallel computing algorithm. Sec. 4 demonstrates and discusses the simulation results for 1D and 2D submicron $n^+ - n - n^+$ structure. Sec. 5 draws the conclusions and suggests the future works.

2 The Poisson-Boltzmann Transport Equations

Due to the ongoing miniaturization in the design of devices mesoscopic models using kinetic transport equations for a distribution function describing the state of the electron gas become more and more relevant: (1) the effects of impact-ionization, (2) tunneling, and (3) hot-carrier transport play an important role in the design of reliable small-scale devices. Therefore it is of paramount importance to describe these phenomena with a TCAD tool [4].

The semiclassical BTE with the Poisson equation for the electric field is the starting point for a rigorous theory. The analytical solution of such a system is impossible from the practical point of view, and for this reason the MCM numerical algorithm has been developed. The MCM is able to describe the behavior of small semiconductor devices even far from thermal equilibrium, because it does not make any restrictive artificial assumptions on the dynamics. Furthermore, the full band structure of the semiconductor and the physical scattering rates can be taken into account. Simulating nanometer size transistors requires solving an integro-differential 5D BTE coupled with the Poisson equation for electron transport. The BTE can be express as follows [9,11],

$$\frac{\partial f}{\partial \tau} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{h} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left( \frac{\partial f}{\partial \tau} \right)_{\text{coll}},$$

where $f = f(\mathbf{r}, \mathbf{k}, \tau)$ is the particle density distribution function in the momentum space at time $\tau$ and location $\mathbf{r} = (r_x, r_y, r_z)$. The $\mathbf{v} = (v_x, v_y, v_z)$ is the particle velocity, $\mathbf{r}$ is the position coordinate in phase space, $\mathbf{k} = (k_x, k_y, k_z)$ is the crystal momentum coordinates in phase space. The term $\mathbf{F}(\mathbf{r})$ is the external force on the particle at location $\mathbf{r}$. The collision term on the right hand side is

$$\left( \frac{\partial f}{\partial \tau} \right)_{\text{coll}} = -\int [f(\mathbf{r}, \mathbf{k}) - f(\mathbf{r}, \mathbf{k}')] \cdot S(\mathbf{r}, \mathbf{k}') \, d\mathbf{k},$$

where the $S(\mathbf{k}', \mathbf{k})$ is the particle transition rate due to scattering mechanism. In many ways, it is similar to the BTE of neutron transport as well as rarefied gas dynamics, but for electrons transport in nanometric structures, there are some added complexities.

![Fig. 1. A 2D cross section view (above) and 1D plot along x or y direction (below) for a $n^+ - n - n^+$ structure.](image)

As shown in Fig. 1, the P-BTE model is subject to mixed type boundary conditions in 1D or 2D a simulation domain. On the source and drain contacts, the Dirichlet type boundary condition is applied for the electrostatic potential. We assume the boundary conditions for particles obeying the conservation law.

Both of the micro- and macroscopic quantities, such as the distribution function, mean velocity, and temperature can be evaluated by statistical methods. The computed distribution function $f$ can be used for the macroscopic physical quantities calculation. We apply the following formula for macroscopic electron density calculation

$$n(\mathbf{r}, \tau) = \int f(\mathbf{r}, \mathbf{k}, \tau) d\mathbf{k},$$
use Eq. (4) to calculate the average electron velocity
\[
\langle \vec{v}(\vec{r}, t) \rangle = \frac{1}{n} \int \vec{v}(\vec{r}, \vec{k}, t) d\vec{k},
\]  
(4)
and follow Eq. (5) to calculate the average electron energy
\[
\langle E(\vec{r}, t) \rangle = \frac{1}{n} \int E(\vec{r}, \vec{k}, t) d\vec{k},
\]  
(5)
where \( n \) is solved with Eq. (3).

In the simulation we consider here the parabolic band structure \( E(\vec{k}) = h^2 \vec{k}^2 / 2m' \) and velocity of the particle is evaluated with \( h \vec{k} / m' \). The scattering mechanisms applied here consist of: (1) acoustic phonon scattering, (2) optical phonon scattering, (3) ionized impurity scattering, and (4) virtual scattering [5]. The BTE is coupled with the Poisson equation for the electric field
\[
\nabla \cdot \vec{E} = \varepsilon_0 \frac{\partial \phi}{\partial t} = q(n - p + D),
\]  
(6)
where the function \( D = -(N^+_{\text{D}} - N^+_{\text{A}}) \) is the specified ionized net doping profile.

3 Adaptive Monte Carlo Method

The conventional MCM consists of a simulation of the motion of electrons (and holes) inside the crystal, subject to the external and self-consistent electric field and of given scattering mechanisms [11]. The simulation starts with electrons in a given initial conditions for momentum and positions. During the free flight, the external forces are made to act according to the usual Newton's law. Then the scattering mechanism is chosen as responsible for the end of the free flight, according to the relative probabilities of all possible scattering mechanisms. From the differential cross section of this mechanism a new state after scattering is randomly chosen as initial state of the new free flight. The Poisson equation is solved to obtain the new electric field and the entire process is iteratively repeated. In this way a stochastic solution to the BTE is obtained. By running this procedure, the carrier history of each particle is recorded and one obtains information on some quantity, such as the distribution function, drift velocity, mean energy, and temperature stress tensor by taking the average of that quantity during the carrier histories in a time interval.

Various P-BTE device modeling and simulation have been developed for the approximation solution on a structured mesh and have their advantages [5-11]. However, the extensive computation required makes it impractical for a device design on a regular basis. Concerning the computational efficiency, we present our adaptive MCM for the P-BTE model simulation. We state the adaptive computing algorithm and the parallelization procedure for the P-BTE Monte Carlo simulation. It relies on the estimations of the solution gradient and variation of carrier lateral current density along the device channel surface. We outline the simulation procedure for the MCM simulation on 1-irregular mesh.

Algorithm 1. (Adaptive single-particle Monte Carlo simulation method for P-BTE model)

1. Compute the maximum of total scattering rate.
2. Initialize the physical quantities for all particles.
3. Determine the free flight time of the particle.
4. Determine each particle location and its electric field with unstructured mesh data.
5. Calculate each particle's momentum and energy before the collision.
6. Determine the scattering process.
7. Compute motion angles \( \theta \) and \( \phi \) after the collision.
8. Calculate their momentum and energy after the collision.
9. After performed the simulation for all particles, we solve the Poisson equation with the adaptive computing algorithm. Otherwise return to Step 3.
10. Update the electric field for all unstructured mesh.
11. Stop the iteration loops and perform the post-processing, if the number of iterations is greater than a specified stopping iteration counts.

The adaptive computing algorithm applied in Step 9 above is followed our earlier works [12-18] and is summarized in Alg. 2. We utilize this algorithm to solve the Poisson equation in 1D/2D structure.

Algorithm 2. (Adaptive computing algorithm for the Poisson equation)

1. Model formulation for the Poisson equations.
2. Domain discretization.
3. Finite volume approximation.
4. System of the corresponding nonlinear algebraic equations: \( \mathbf{Ax} = -\mathbf{F(x)} \).
5. The MI nonlinear solver.
6. A posteriori error estimation.
7. Mesh refinement.

If the estimator is less than a preset error tolerance, the process will be terminated and the approximated solution can be post-processed for next iterations. Otherwise, our refinement scheme will refine the mesh using the maximum gradient of electrostatic potential \( \phi \) and the variation of current density \( J \), as error estimation. The proposed parallel computing procedure for accelerating the MCM execution speed is outlined in the following algorithm. Alg. 3 is based on the partition of total particles numbers.
Algorithm 3. (Parallel computational procedure)
Step 1. Initialize the MPI and configurations.
Step 2. Setup unstructured mesh dynamical array structure.
Step 3. Count number of particles and apply a dynamic MCM partition algorithm to determine number of processors in the simulation.

Algorithm 3.1. (dynamic MCM partition algorithm)
Step 1. Count the number of total particles.
Step 2. Find out the optimal number of processors.
Step 3. Determine how many particles should be assigned to each processor.
Step 4. Along x- or y-direction in device domain, search (from left to right and bottom to top) and assign particles to these processors sequentially.
Step 4. All assigned CPUs perform the MCM simulation with Alg. 1.

4 Simulation Results and Discussion
We present simulated results; the simulation example is a 1D 0.4μm n+-n-n+ semiconductor structure with 0.2 μm source and drain contacts [1]. The applied voltage V_D is fixed at 2 V. The simulation consists of 50000 particles more than 100000 iteration loops to reach the self-consistent solution.

Fig. 2. The device doping profile and its electron density at V_D = 2.0 V.

Fig. 3. The corresponding gradient of the electron density.

Fig. 4. The simulated electrostatic potential for the n+-n-n+ structure at applied voltage 2.0 V.

Fig. 5. The computed electric field for the n+-n-n+ at 2.0 V.

Fig. 6. A plot of the simulated average electron velocity.

Fig. 2 shows the simulated electron density, where the solid line is the specified doping profile and the dot one is the corresponding electron density in log scale. Fig. 3 shows the electron density variation between the junctions. Our adaptive scheme successfully locates the solution variation. We plot the potential distribution and electric field in Figs. 4 and 5, respectively. Compared with the Fig. 10, the computed electric field provides a very good error control scheme and mesh refinement indicator.
We plot the calculated average electron velocity, energy, and temperature in Figs. 6, 7, and 8, respectively. The results demonstrate the device has higher electron temperature near the drain side. The electron attains the maximum velocity and energy in the drain junction neighborhood.

Furthermore, Fig. 9 is a comparison of the device I-V curve between the analytical formula [1] and simulation result, and shows its accuracy of the modeling and simulation. We report the adaptive and parallel performance for the parallel adaptive simulation approach in Figs. 10, 11, and 12, respectively. As shown in Fig. 10, the 1D refinement is with a refinement criterion on the potential. Figs. 11 and 12 are the achieved parallel speedup and efficiency on a 16-PCs Linux-cluster.

Fig. 7. A plot of the simulated average electron energy.

Fig. 8. The simulated average electron temperature.

Fig. 9. The I-V curve for the n+-n-n+ structure at 2.0 V.

Fig. 10. Refinement levels for the 1D model problem.

Fig. 11. The achieved parallel speedup for the problem.

Fig. 12. The parallel execution time and parallel efficiency for the n+-n-n+ structure simulation.

Besides good parallel efficiency and speedup are reported, Figs. 13 and 14 present the adaptive refinement efficiency for a 2D n+-n-n+ model problem. As shown in Fig. 14, we use the electron density gradient as the refinement mechanism. It is different from our 1D refinement approach, but the
refinement behavior has good agreement with the 1D simulation result as shown in Fig. 3.

![Figure 13](image1.png)

**Fig. 13.** Initial mesh for the 2D n+-n- structure simulation.

![Figure 14](image2.png)

**Fig. 14.** A refined mesh for the 2D n+-n- structure at applied voltage: 2.0 V.

## 5 Conclusions

We have presented an adaptive 1-irregular mesh simulation technique for the Monte Carlo solution of semiconductor Poisson-Boltzmann transport equations on a Linux-cluster. Our MCM approach was based on adaptive 1-irregular mesh, monotone iterative method, and a posteriori error estimation method. The coupled Poisson Eq. and BTE were solved with Monte Carlo method on an unstructured mesh for 1D/2D n+-n- device. It had more computational efficiency than the conventional simulation on structured mesh. Furthermore, our simulation not only showed the novelty and robustness of the method but also demonstrated it can be utilized for multi-dimensional nanometer scale device simulation.

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