A Simple and Efficient Method for the Calculation of Carrier-Carrier Scattering in Monte-Carlo Simulations

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Abstract—**The analysis of the carrier-carrier scattering is getting more important and it can be done by the particle-particle-particle-mesh (P^3M) algorithm. A problematic part of the algorithm is to avoid double-counting of the pair forces in short-range. Here, we solve the problem by introducing an efficient numerical method to the algorithm. The improvements in accuracy and applicability are confirmed with various test cases. In addition, the modified P^3M method is integrated with a 3D ensemble Monte Carlo (EMC) simulator and applied to the device simulations. The results are compared with those of the PM (particle-mesh)-EMC approach, which reveals the limitations of the scattering rate based methods and the importance of the P^3M method to treat carrier interactions.**

I. INTRODUCTION

Accurate treatment of carrier interactions is becoming increasingly important as device scaling continues and each individual carrier exerts more influence on overall device performance [1-2]. However, it is well known that the carrier-carrier scatterings are difficult to treat in Monte Carlo simulations [2-4]. In Fermi's Golden Rule based approaches, unlike other scattering rates, the carrier-carrier scattering rates need to be updated during the simulation to account for the local dependence of the distribution function and screening length [2-3]. The process is computationally expensive and it is difficult to account for local variations of the carrier density [3]. One of the alternatives for the analysis of the carrier interactions is the particle-particle-particle-mesh (P^3M) algorithm [1,4,5]. In classical limit, P^3M is the most attractive method since it combines the accuracy of the local particle-particle (PP) force evaluation with the efficiency of the particle-mesh (PM) force evaluation [1,5]. In this way, accurate short-range calculation of charge interaction can be extended to a full device structure with small overhead, beyond the cost already involved with the Poisson equation [5]. Hockney and Eastwood found that the main practical problem associated with the short-range force calculation is to avoid double-counting of pair forces, and they suggested somewhat lengthy analytical solution [5].

In this paper, we introduce an alternative numerical method that is accurate, simple to implement, and that improves the applicability of the P^3M approach to general device simulations. The proposed model is implemented in a P^3M-EMC (ensemble Monte Carlo) simulator for the analysis of the carrier-carrier scattering and the results are compared with those of PM-EMC simulations.

II. METHOD

Monte Carlo based device simulation consists of two self-consistent components. One is transport simulation to calculate the movement of the particles under the influence of electric field. Generally, the influence of carrier scattering is included during the procedure. The other is solving field (Poisson's) equation to obtain driving force for the charge carriers. To some extent Coulomb scatterings such as carrier-carrier and carrier-impurity scatterings can be considered naturally by solving Poisson's equation. Without very fine mesh, however, this PM based method is inherently inaccurate in short range. The P^3M method replaces inaccurate PM force with accurate PP force in short range. In the P^3M approach, the short-range force, F^{sr}, is given by

$$F^{sr} = F^m + F^d - F^r \tag{1}$$

where F^m is the local mesh force introduced by Poisson's solution (PM method), F^d is the direct force by Coulomb's law (PP method), and F^r denotes the so-called 'reference force'. Ideally, F^r should be the same as F^m so as to determine F^{sr} exclusively by F^d. Since there has been no known method to precisely reproduce F^m, approximate analytical solution has been suggested [5]. However, considering the complexity of F^m calculations, the analytical solution is too simple, since it only involves the short-range radius (rsr) and the distance between particles.

The purpose of our work is to obtain a more accurate reference force, F^r, by reverse engineering the PM method. The general PM method consists of four steps as shown in the left flow in Fig. 1. Our numerical scheme, to reproduce local PM force, follows the same procedure with the difference being in the governing equation in second step. After assigning charges of particle i and j to the mesh nodes as in Fig. 2, we evaluate the reference force of particle j on particle i, using

$$F_{ij}^r = \sum_{m \neq n} \frac{w_{i_n} w_{j_m} q_i q_j}{4\pi\varepsilon} \frac{(r_{i_n} - r_{j_m})}{\left| r_{i_n} - r_{j_m} \right|^3} \tag{2}$$

where q is the electron charge, ε is the dielectric constant, w is the fraction of charge, r is the position, and n and m

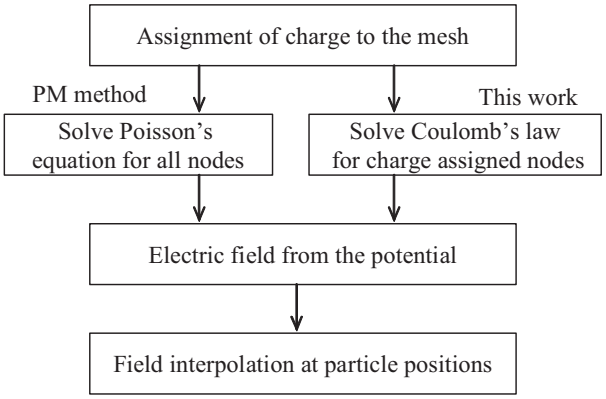
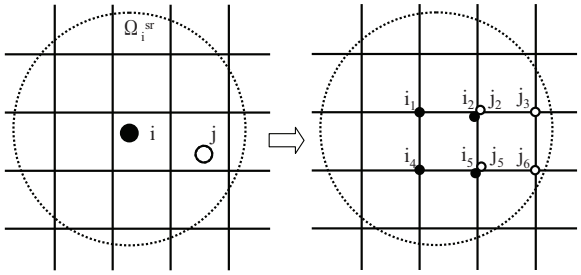


Fig. 1. Flowchart of the PM method and this work to obtain accurate reference force. Instead of solving Poisson's equation on all the mesh nodes, equivalent Coulomb's equation is solved only for the charge assigned mesh nodes.



(a) Particles inside short range (b) Charge assignments

Fig. 2. Charge assignments of the particles inside the short-range (rsr) using the cloud-in-cell (CIC) scheme. For the simplicity, two dimensional example is described and the fraction differences of assigned charge are not precisely illustrated here.

are node indices for the mesh nodes to which the charges of i and j are assigned, respectively.

One of the merits of this method is that, in principle, the reference force should not include external forces, e.g., forces induced by boundary conditions, and this can be done automatically by using Coulomb's law instead of Poisson's equation.

III. Simulation Results

Fig. 3 shows that the proposed numerical model agrees well with the existing analytical solution. We further evaluated the method for more general conditions.

To make standard solutions of the reference force, we employed a 3D Poisson's solver. It is important to note that the 3D Poisson's solver is hard to be used for the regular reference force calculations due to the enormous computational burden. However, it can be used for the evaluation of other methods. Even though the influence of the external forces cannot be eliminated completely in Poisson's solver, the simulation domain was set to be wide enough to minimize it.

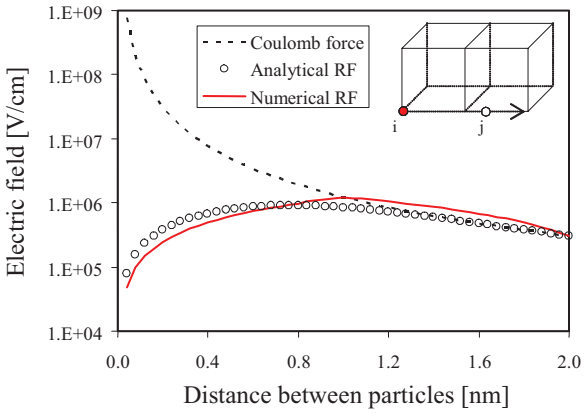


Fig. 3. Reference forces (RF) and the direct Coulomb force are described. Analytical RF is based on the equations in [5]. Numerical RF is from equation (2). CIC scheme is used and rsr is set to 2 meshes (i.e. 2nm). Uniform cubic mesh, 1×1×1nm, is used and the particle i is assumed to be at the mesh node and j is moved along the mesh line. (Note : $Electric\ field = F_{ij}^{r} / q_i$)

We varied the short-range radius (rsr) and charge assignment schemes. The verification results in Fig. 4 and 5 show that the numerical reference forces match well with the solutions of the Poisson's solver for various conditions. This indicates that the numerical method gives us more flexibility in selecting the charge-assignment scheme and short-range radius.

For the application on regular device simulations, the applicability on non-uniform mesh has great importance. The evaluations on non-uniform mesh (see Fig. 6) clearly show the accuracy improvements of the numerical method. The results are reasonable because the numerical method is designed to mimic the PM procedure. The analytical solution also yields reasonable results when the short-range radius corresponds to 2 meshes and uniform cubic meshes are used as in Fig. 4 (b), but it shows large errors in general cases. The implementation of the numerical method to standard P^3M algorithm is expected to widen the application area of the algorithm.

Following the evaluation, the modified P^3M algorithm was integrated into a 3D EMC simulator. The device simulations were performed for a surround-gate-transistor (SGT) with 60nm length, 20nm body thickness, and 1V supply voltage. The device simulation results were compared with those of the PM-EMC method, which is important because an alternative scattering rate approach is based on the PM method. Accordingly, the properties of the PM method directly affect the scattering rate approaches.

During the carrier interactions, the total energy of the carriers should be conserved. In Fig. 3, we can notice that the PM force approaches zero as the distance of the two carriers decreases, even though the real force should be as strong as Coulomb's force. This implies that the energy of the carriers will decrease during the carrier-carrier interactions as we increase the size of the mesh.

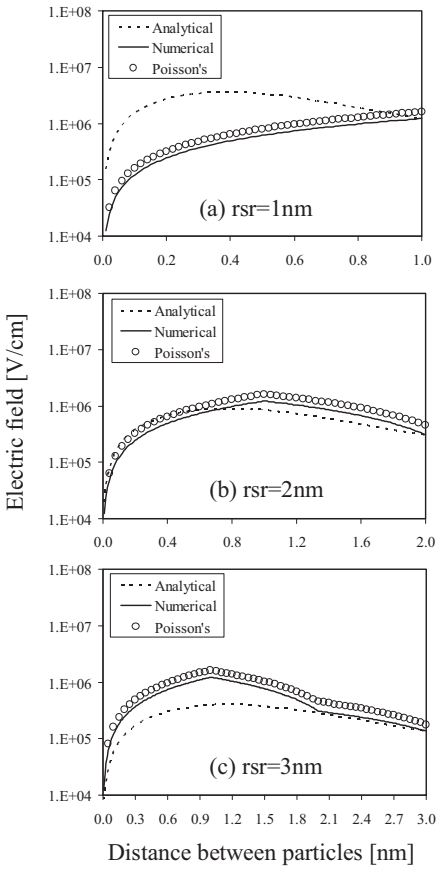


Fig. 4. Comparison of the reference forces for various rsr. CIC is used for the charge assignment scheme. The relatively small discrepancy between the numerical reference force and Poisson solution is due to the truncation error of the Poisson's solution.

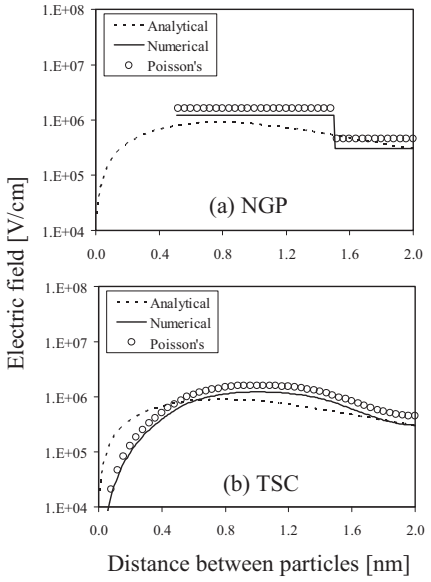


Fig. 5. Comparison of the reference forces for various charge assignment schemes. (Note : NGP-nearest grid point, TSC-triangular shaped cloud)

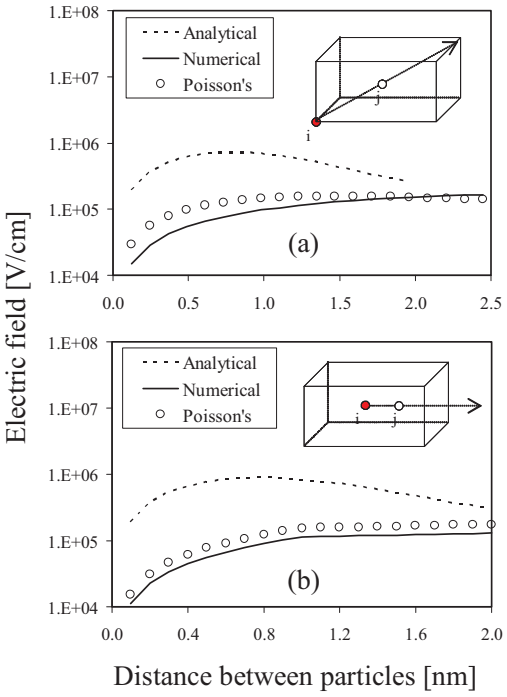


Fig. 6. Evaluation on the non-uniform mesh, 2×1×1nm, applications. (a) particle i is at the mesh node and j is moved along the diagonal direction. (b) particle i is at the center of the cell and j is moved along the center line.

In order to verify the assumption, we performed the simulations with various mesh sizes. Fig. 7 (a) and (b) compares the distribution functions of PM-EMC and P^{3}M-EMC method. In the case of PM-EMC, as expected, the number of carrier with high energy is decreased as we increase the size of the mesh. On the other hand, for P^{3}M-EMC, the variation is reduced significantly. The corresponding quantitative average energy of the carriers and on-currents of the SGT are described in Fig. 8.

Unlike PM-EMC, the average energy and on-current of P^{3}M-EMC are conserved for wide range of mesh size. Fig. 8 also indicates that the PM-EMC can be as accurate as the P^{3}M-EMC with very fine mesh applications, however, it is computationally expensive as shown in Fig. 9. Comparison of simulation time between PM-EMC and P^{3}M-EMC also shows that despite extra calculations on the P^{3}M method, the increase of simulation time is marginal. Considering the results of Fig. 8 and 9, we can estimate that the computational time can be reduced by 80~90% by using proposed P^{3}M-EMC without the sacrifice of the accuracy.

IV. CONCLUSIONS

A numerical method is introduced to replace the analytical method of the P^{3}M algorithm. Accuracy and applicability of the P^{3}M method are improved by the proposed method which effectively eliminates double-counting of the short-range

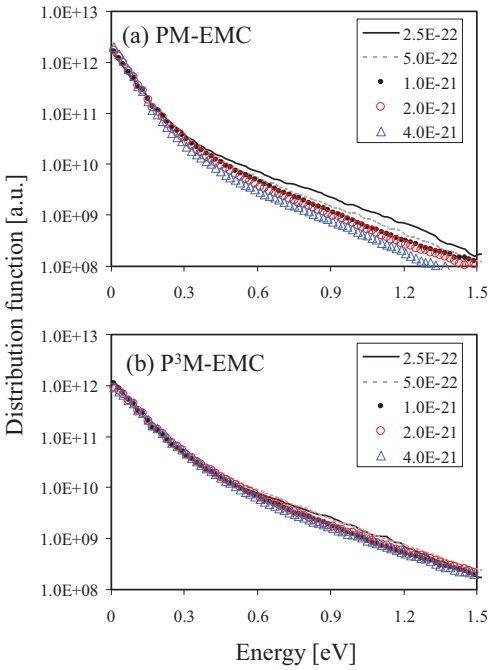


Fig. 7. Distribution functions for (a) PM-EMC and (b) P^3M-EMC with various mesh sizes [cm^3]. Considerable changes are observed for the PM method. Distribution functions for P^3M also show some variations but the improvement is evident.

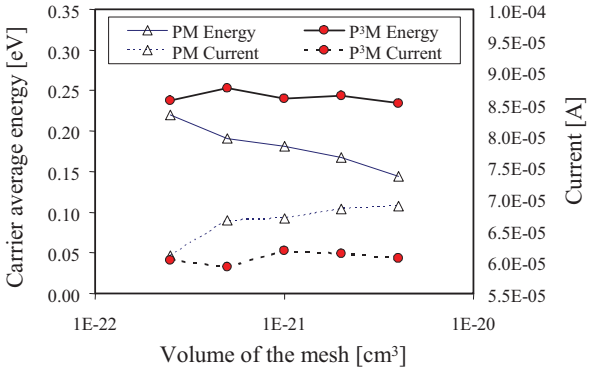


Fig. 8. Average energy of the carriers and the corresponding on-currents of the SGT are shown. Decrease of average energy in PM-EMC reduces the scattering rates, e.g., optical phonon scattering, and which leads to the increase of on-current.

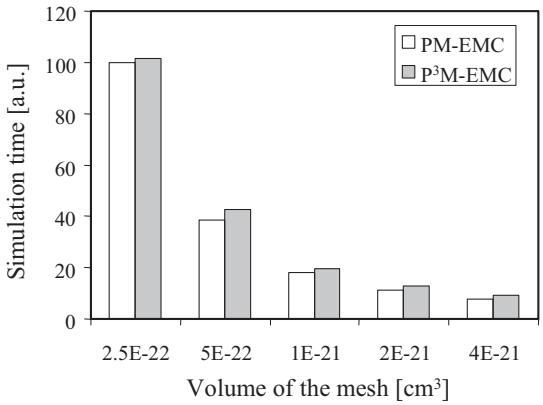


Fig. 9. Simulation time as a function of mesh size [cm^3]. The simulation time can be reduced significantly by using coarse mesh combined with P^3M-EMC approach. For the same size of the mesh, simulation time of P^3M-EMC is close to that of PM-EMC because the simulation time is mainly determined by the calculation of 3D Poisson's equation.

forces in various conditions. The modified P^3M method is combined with the EMC simulator and compared with the PM-EMC simulator. Applications on the device simulation reveal the limitations of the PM-EMC based scattering rate approach and the advantages of the P^3M-EMC method for the calculation of carrier interactions.

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