Efficient Simulation of the Full Coulomb Interaction in Three Dimensions

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The continued scaling of MOSFETs into the nano-scale regime requires refined models for carrier transport due to, e.g., unintentional doping in the active channel region which gives rise to threshold voltage and on-state current fluctuations. Therefore every transport simulator which is supposed to accurately simulate nano-devices must have a proper model for the inclusion of the Coulomb interactions. In a typical Poisson–MC transport simulation sequence the long range portion of the Coulomb interaction (due to both the electron-electron and the electron-impurity interactions) is included via the repeated solution of the Poisson equation. The short range part of the interactions is included in the k-space portion of the MC transport sequence. This approach is impractical and inaccurate for the following two reasons.

First the separation of the Coulomb interaction in a short and long range component is inaccurate and the long range part may depend on the mesh size. Second the k-space treatment of the short range part is inaccurate, since it is necessary to know the distribution function to accurately describe the screening. The evaluation of the distribution function is in turn rather CPU intensive and noisy because of the poor statistics usually found in realistic device structures. Hence a real space treatment of the short range interactions has been proposed. Variants thereof are the P^3M (particle-particle particle-mesh) method [1] and the corrected Coulomb approach [2]. Although real space treatments eliminate the problem of double counting the force, a drawback is that the Poisson equation must be solved repeatedly to properly describe the self-consistent fields, which consumes over 80% of the total simulation time in three dimensions.

To avoid all of the above mentioned issues and to further speed up simulation time, we propose to use a 3D FMM (fast multi-pole method) [3, 4] instead. The FMM is based on the idea of condensing the information of the potential generated by point sources in series expansions. After calculating expansions in a hierarchical manner, the long range part of the potential is obtained by evaluating the series at the point in question and the short range part is calculated by direct summation. Its computational effort is only $O(n)$ where n is the number of particles.

In order to validate the physical corrected and speed of the FMM approach, we first simulate an n^+–n–n^+ resistor. The theoretically calculated results for the low field electron mobility using the P^3M, the corrected Coulomb, the FMM, and the Brooks–Herring k-space approach are compared with available experimental data [5] in Figure 1. It is found that the low field mobility calculated with the FMM approach agrees very well with the experimental values for both low and high field doping concentration. The k-space Brooks–Herring approach significantly overestimates the low field electron mobility for high substrate doping densities. The simulation times were halved when using the FMM compared to the P^3M approach.

We have also tested the speed of the FMM approach on the example of a 3D SOI device structure shown in Figure 2 using both the Hartree or particle-mesh (PM) and the FMM approach. The field due to the boundary conditions is also shown in this figure. The device drive current and the average carrier energy are shown in Figure 3 for a preset value of the gate and the drain bias. The difference in the I_d–V_d curve is due to the omission of the short range Coulomb interaction in the PM approach. Also the use of the FMM leads to faster decay of the carrier energy which suggests that the short range interactions are responsible for the thermalization of the carriers entering the drain reservoir. Here the total simulation times were decreased by a factor of ≈ 20 when using the FMM, i.e., from ≈ 20 hours to a less than an hour on current hardware.

In summary the use of the FMM approach for semiconductor transport simulations was validated. Simulation times are decreased significantly and effects due to electron-electron and electron-impurity interactions are observed as expected. Since the FMM algorithm operates independently of the grid used in the MC simulation, it can be easily included into existing MC device simulation codes.

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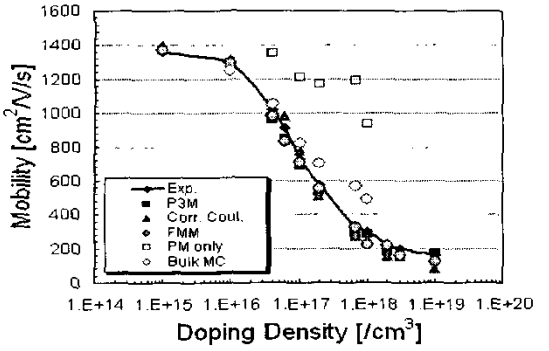

Method	Average time per iteration	Total Time (400 iterations)
P^3M	35 s	233 min
FMM	17 s	113 min

Figure 1: Results of three-dimensional simulations for the n^+–n–n^+ resistor (360 nm · 50 nm · 50 nm). **Left:** The electron mobility for five doping concentrations (from $10^{15}\,\mathrm{cm}^{-3}$ to $10^{19}\,\mathrm{cm}^{-3}$) as obtained experimentally and by five simulation methods. **Right:** The simulation times on a 600 MHz Pentium III computer. The total number of charges is $\approx 22\,000$, and the MC mesh size is $50 \cdot 20 \cdot 20$.

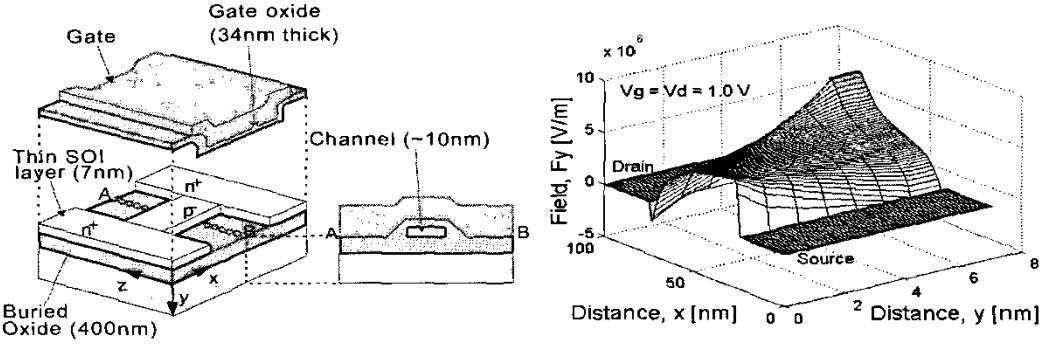

Figure 2: Left: The device structure of the 10 nm SOI MOSFET. **Right:** The y-component of the field due to the boundary conditions, F_y, within in the device for $V_g = V_d = 1.0\,\mathrm{V}$.

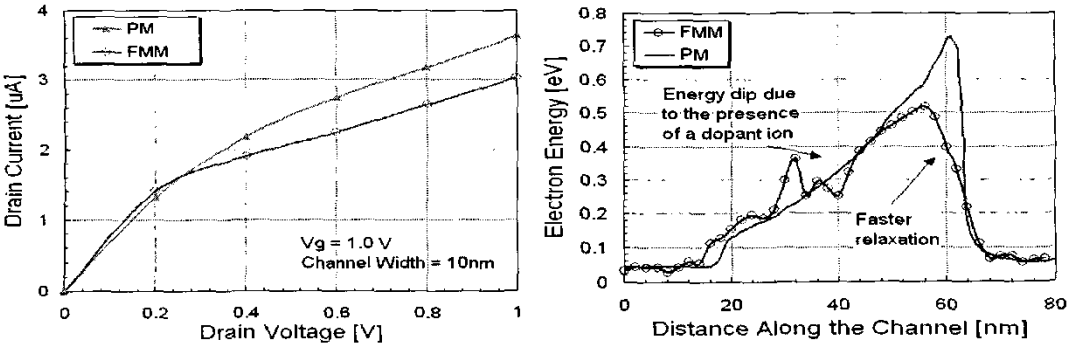

Figure 3: Left: The I_d–V_d curve for a gate voltage of $V_g = 1.0\,\mathrm{V}$ as obtained by the PM and FMM methods. **Right:** The electron energy along the channel for the PM and FMM approaches.

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