

# On the efficient simulation of electron-electron interactions in nanoscale MOSFETs

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**Abstract.** The full Coulomb interaction, i.e., electron-electron and electron-impurity interactions are going to play an increasingly important role in nanoscale MOSFETs. Previously these effects were usually simulated by particle-particle particle-mesh and corrected Coulomb methods which were found to be very time consuming. In this paper we propose to use a fast multi-pole method instead. This enables to decrease simulation times significantly and it was verified in several nanoscale device simulations that the simulation results are physically correct. We describe the simulator used and compare the results obtained by the fast multi-pole method to previous approaches. Due to the advantages of the fast multi-pole method we expect it to replace previous approaches used in particle-based EMC codes for semiconductor device simulation.

## 1. Introduction

The constant need for integration of more functions on a chip necessitates continuous scaling of the semiconductor devices. According to the SIA road-map for semiconductors it is expected that by 2014 production devices will have a gate-length of 35 nm and a oxide thickness of less than 1 nm. There are, however, a number of barriers that have to be overcome in accomplishing this goal.

One issue that will pose serious problems in circuit operation are the transistor mismatches due to the different number and different patterns of the impurity atoms underneath the gate. This will affect the off-state current and the device threshold voltage. Hence there are significant fluctuations in the threshold voltage from device to device fabricated on the same chip. The solution to this problem is to use undoped silicon films. However unintentional doping, i.e., the presence of even a single impurity atom, can significantly alter the performance of the device under consideration.

The full Coulomb interaction will have a major impact on device characteristics in ultra-small MOSFETs because of the small number of electrons in the channel and the long-range properties of the Coulomb force. Electron-electron and electron-impurity interactions affect the threshold voltage, the carrier dynamics, and the device characteristics [4, 6].

Now the continuous scaling of MOSFET devices into the nanoscale regime requires refined models for electron transport. Coulomb interactions must be considered because of two reasons. First the Coulomb force is a long range force implying that both the short and the long range interactions must be included in a particle ensemble. Second the hot-carrier and short-channel effects will have a significant impact on device performance due to the small number of carriers and impurities in the active region of nanoscale devices.

Most Ensemble Monte Carlo (EMC) simulators however do not include the full Coulomb interactions due to the necessary computational time and resources. Yet two techniques have been used in the past for properly including the short and the long range electron-electron and electron-ion interactions in particle based simulations: P<sup>3</sup>M (particle-particle particle-mesh) methods [8], adapted to the boundary conditions necessary for semiconductor devices, and the corrected Coulomb approach [4, 5, 6]. However both approaches suffer from drawbacks when used in the context of transport simulations in semiconductors.

To overcome these problems we propose to use a FMM (fast multi-pole method) [3, 1, 2, 7], as summarized in the next section, instead. For our applications this means that all Coulomb field effects can be included while avoiding the long computation time of the P<sup>3</sup>M method.

After describing the simulation methods in more detail, we calculate the electron mobility in silicon using five different methods in the examples section and compare the results to experimental values.

## 2. Simulation Method

In this section we discuss the three main simulation methods and the EMC simulator.

### 2.1. The PPPM Method

P<sup>3</sup>M methods work by splitting the potential into two parts: the short range interactions, which are obtained by direct evaluation, and the long range interactions, which are handled by distributing the sources onto a grid and solving the Poisson equation on this grid. For a given particle the potential is evaluated by summing the short range and long range part and subtracting the influence of nearby particles in the long range part in order to prevent taking nearby particles into account twice.

P<sup>3</sup>M methods are mainly used in astrophysical simulations and quantum chemistry. However, when they are applied to simulations of semiconductor devices, there are some drawbacks. Firstly DFT cannot be used to solve the Poisson equation since the boundary conditions are non-periodic, whereas periodic boundary conditions are commonly used for astrophysical problems.

Secondly the inverse of the Laplace operator must be calculated for each particle in order to prevent counting nearby particles twice which is, of course, very time consuming. In order to alleviate this problem the inverse can be precomputed (which takes several hours) and stored (which requires lots of memory), but this must be repeated for every new device structure.

Thirdly the separation of the Coulomb interaction in a short and a long range component is inaccurate and the long range part may depend on the mesh size. Non-uniformity in the source distributions can cause degradation of performance and errors may originate from the numerical differentiation used to calculate the field from the mesh potential depending on the scheme to couple a particle to the mesh. Secondly 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.

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 time spent in 3D simulations.

### 2.2. The Corrected Coulomb Approach

The corrected Coulomb approach [4, 5] is a purely numerical scheme that generates a corrected Coulomb force look-up table for the individual electron-electron and electron-ion interaction terms. To calculate the proper short range force one defines a 3D box with uniform mesh spacing in each direction. A single (fixed) electron is then placed at

a known position within the 3D domain, while a second (target) electron is swept along the domain in small increments so that it passes through the fixed electron.

The 3D box is usually made sufficiently large so that the boundary conditions do not influence the potential solution. The electron charges are assigned to the nodes using one of the charge assignment schemes. A 3D Poisson equation solver is then used to solve for the node or mesh potentials. At self-consistency the force on the swept electron  $F = F_{\text{mesh}}$  is interpolated from the mesh or node potential.

In a separate experiment the Coulomb force  $F_{\text{tot}} = F_{\text{coul}}$  is calculated using the standard Coulomb law. For each electron separation one then tabulates  $F_{\text{mesh}}, F_{\text{coul}}$  and the difference between the two  $F_{\text{sr}} = F_{\text{coul}} - F_{\text{mesh}}$ , which is called the corrected Coulomb force or the short range force. The latter is stored in a separate look-up table.

It is clear that the mesh force and the Coulomb force are identical when the two electrons are separated by several mesh points. Therefore adding the two forces in this region would result in double counting of the force. Within three to five mesh points  $F_{\text{mesh}}$  starts to deviate from  $F_{\text{coul}}$ . When the electrons are within the same mesh cell, the mesh force approaches zero due to the smoothing of the electron charge when divided amongst the nearest node points. The generated look-up table for  $F_{\text{sr}}$  also provides important information concerning the determination of the minimum cut-off range based upon the point where  $F_{\text{coul}}$  and  $F_{\text{mesh}}$  begin to intersect, i.e., where  $F_{\text{sr}}$  goes to zero.

### 2.3. The FMM Approach

The FMM is based on the idea of condensing the information of the potential generated by point sources in several truncated series expansions. After calculating suitable expansions, the long range part of the potential is obtained by evaluating the truncated 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, instead of proportional to  $\binom{n}{2}$  for direct summation.

For 3D simulations we used the standard Coulomb potential. Note that in two dimensions the Coulomb potential at a point  $x \in \mathbb{C}$  produced by a point electric charge  $q_0$  at  $x_0 \in \mathbb{C}$  is given by

$$\Phi(x) = -\frac{q_0}{2\pi\epsilon} \text{Re}(\log(x - x_0)).$$

This two-dimensional potential is obtained by postulating that (1) the Coulomb force is a long range force and that (2) Gauss' law holds. The approximation to the field can be obtained by numeric differentiation.

Using the PM (particle-mesh) approach, the electric field due to the dopants and the applied boundary biases was obtained at the start of the simulation by solving the Poisson equation. Hence the total field acting on each electron is the sum of this constant field and the contribution from the electron-electron interaction handled by the FMM calculations.

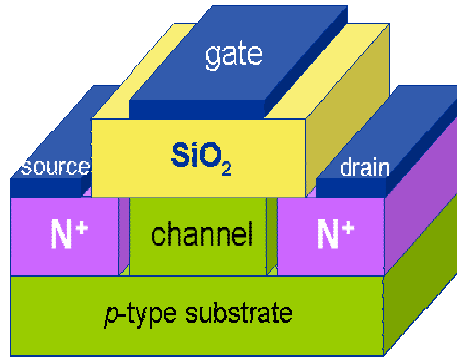


Figure 1. Device structure.

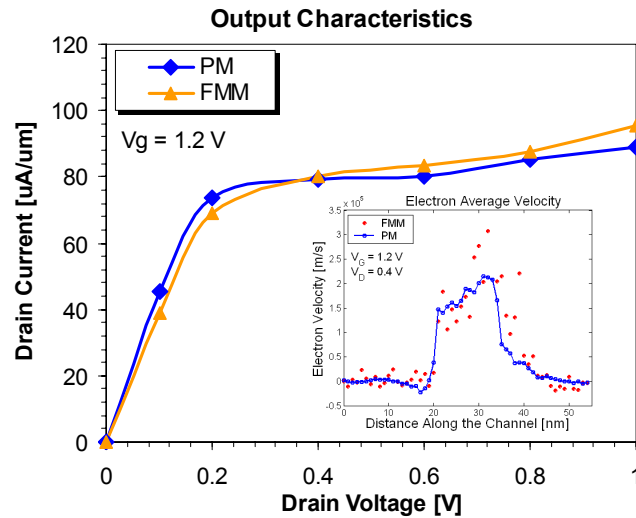


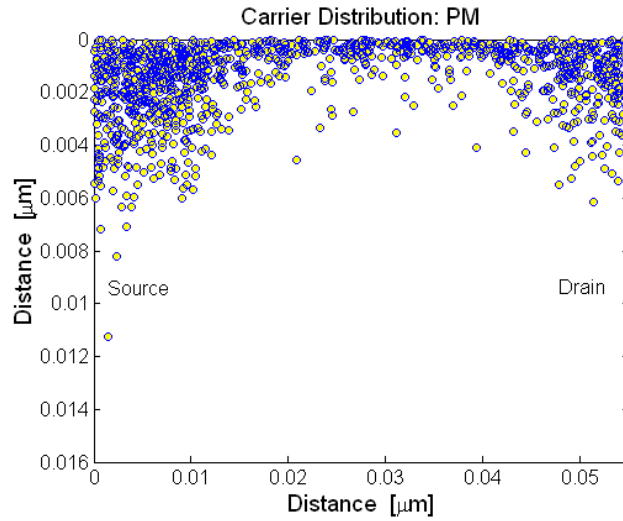
Figure 2. The output characteristics for  $V_G = 1.2$  V.

#### 2.4. The 3D Ensemble Monte Carlo Simulator

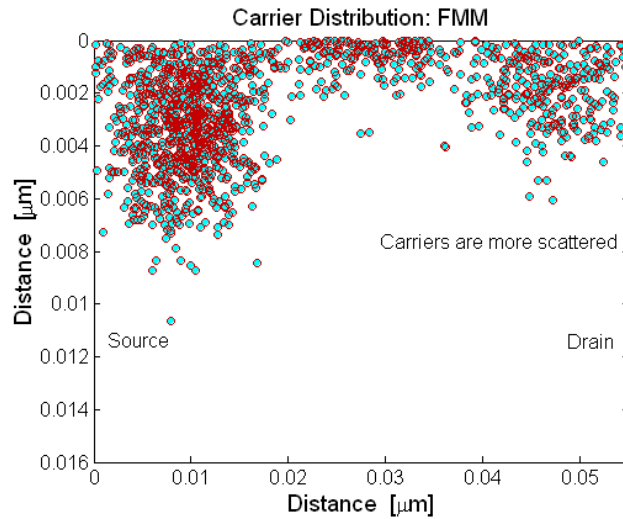
We close this section with a short description of our 3D EMC device simulator. The Monte Carlo transport kernel is based on 3D electrons distributed amongst three equivalent valleys with energy dependent effective masses. In the  $k$ -space portion of the MC transport kernel we have included acoustic and intervalley (g- and f-phonons) scattering processes. Surface roughness is included as a real-space scattering process. We assume 50% to be specular and 50% to be diffusive reflections from an ideal atomically flat interface.

### 3. Simulation Results for a 15nm MOSFET

In order to verify that this approach is advantageous for particle based EMC simulations, we used it to study the effects mentioned above in a MOSFET with a gate length of 15 nm using our EMC simulator.



**Figure 3.** The electron distribution along the channel as obtained by the PM method.

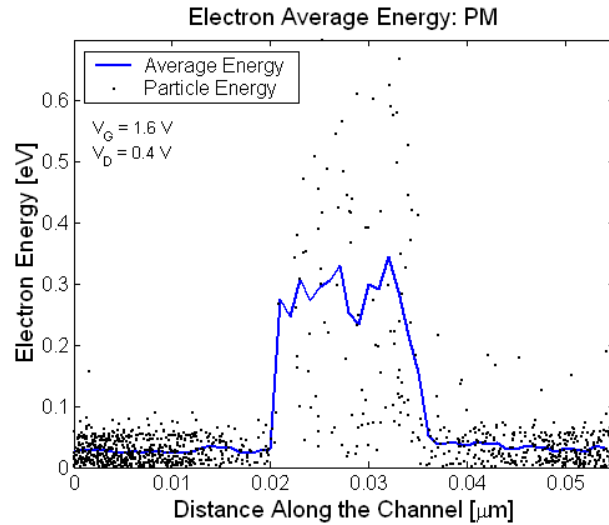


**Figure 4.** The electron distribution along the channel as obtained using the FMM approach.

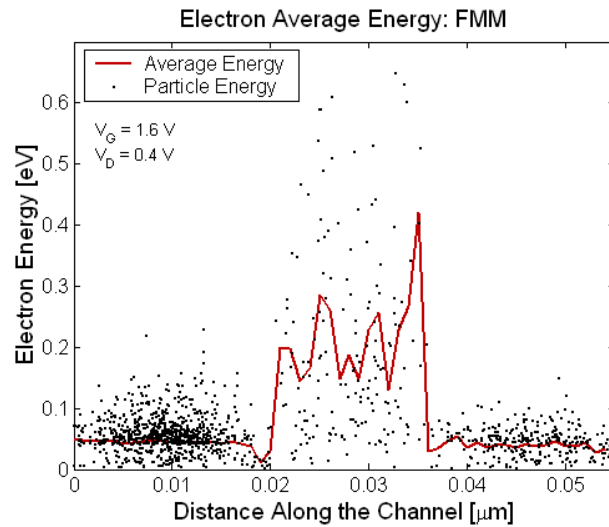
The simulated device is shown in Figure 1 and has an oxide thickness of 1.0 nm, a channel length of 15 nm, a channel width of  $0.5 \mu\text{m}$ , a source-drain junction depth of 15 nm, and the substrate doping is  $N_A = 3 \cdot 10^{19} \text{ cm}^{-3}$  and the doping of the source-drain regions is  $N_D = 10^{19} \text{ cm}^{-3}$ .

The electric field due to the long-range electron-ion interaction and the applied boundary biases was calculated once in the beginning by solving the Poisson equation.

The output characteristics of the device for  $V_G = 1.2 \text{ V}$  are shown in Figure 2. The inset shows the average electron velocity along the channel for  $V_G = 1.2 \text{ V}$  and  $V_D = 0.4 \text{ V}$ . The current increase in the FMM case can be attributed to the increase in carrier velocities in the channel region. We see that the use of the FMM approach



**Figure 5.** The average electron energy along the channel for the PM case for  $V_G = 1.6$  V and  $V_D = 0.4$  V.



**Figure 6.** The average electron energy along the channel for the FMM case for  $V_G = 1.6$  V and  $V_D = 0.4$  V.

gives rise to slightly degraded device transconductance at low drain voltages, but at high drain voltages, when there is a large number of electrons in the channel region of the device, the FMM and the PM approach lead to almost the same amount of current, but different output conductance.

The electron distributions in the device obtained by the PM and the FMM approach are shown in Figures 3 and 4. We observe that the inclusion of the short range interactions leads to more scattered electrons. We also have to note that the artificially large force that results when two electrons are very close to each other was eliminated by introducing a proper cut-off range. Finally we show the energy characteristics along

the channel region in Figures 5 and 6.

There are several noteworthy features that can be observed when analyzing this data. Firstly the inclusion of the electron-electron interactions leads to fast thermalization of the carriers at the drain end of the device. Secondly the average electron energy and the average electron velocity increase when using the FMM approach, i.e., when including the short range electron-electron interactions. In summary the results presented in this work suggest that electron-electron interactions, namely both the short and the long range components, must be properly included when modeling nanoscale MOSFETs.

#### 4. Conclusion

Since FMM implementations are independent of any grids possibly used during the MC part of the simulation, it can be included into existing MC device simulation codes in a straightforward manner. In summary simulation times are significantly reduced and the simulation results agree better with experimental data than previously used methods while accounting rigorously for short range and long range electron-electron and electron-ion interactions.

The careful treatment of electron-ion and electron-ion interactions is a premise for the realistic simulation of nanoscale MOSFETs. Unintentional doping leads to considerable fluctuation in the device parameters. Furthermore the electron-electron interactions affect the thermalization of the carriers at the drain end of the device. Impurities near the middle portion of the source end of the channel have most significant impact on the device drive current. Regarding the electron-electron interactions it was found that they affect the carrier velocity near the drain end of the channel.

Simulation times are an important issue for MC simulations. The simulation of the characteristics of a device is especially tedious considering that previously one simulation took about a day. The speed-up observed in the FMM simulations will facilitate the exploration of future devices and new device structures.

#### 5. Acknowledgment

The first author acknowledges support by the Austrian Science Fund (Fonds zur Förderung der wissenschaftlichen Forschung, FWF) via an Erwin Schrödinger Fellowship. The authors also acknowledge support from NSF under contract No. ECS 021-8008.

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