

# Convergence Properties of Density Gradient Quantum Corrections in 3D Ensemble Monte Carlo Simulations

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*Abstract*—A methodology to include quantum corrections in 3D Monte Carlo simulations is presented, based on the Density Gradient formalism. Three flavours are introduced, with increasing degrees of self-consistency between the current, field and quantum correction and compared in terms of accuracy and impact on the current voltage characteristics.

*Keywords*—Monte Carlo, quantum corrections, Density Gradient

## I. INTRODUCTION

The continued scaling of MOSFETs with both conventional and novel architectures enhances the role of non-equilibrium transport and quantum phenomena requiring increasingly detailed and complex simulation techniques. Most of the now widely researched multigate devices are 3D in nature and thus require full scale 3D simulations [1]. 3D simulations are also a necessity when studying statistical device variability introduced by discreteness of charge and matter [2]. The Monte Carlo (MC) approach offers a compromise between the computationally efficient but oversimplified Drift Diffusion (DD) technique [3], and cumbersome full-scale quantum transport simulations [4] in the 3D simulation domain. 3D MC simulations are also a necessity when studying transport variability due to scattering from the unique surface roughness and body thickness patterns [5] and the random discrete dopants in nanoscale CMOS devices [6]. Inherently semi-classical in nature, the MC approach can be enhanced by the introduction of quantum corrections with a different level of sophistication and accuracy. Typically, quantum effects are introduced into MC via corrections applied to the driving force [7]. Most of the MC quantum correction techniques so far have been developed, demonstrated and restricted to 2D simulations, with the few published quantum correction examples applied in 3D based on the Effective Potential [8] and Schrödinger-based [9] approaches.

Here, we discuss in detail the accuracy and convergence properties of a new flavour of 3D Density Gradient [10] quantum corrections introduced in a fully self-consistent manner to 3D MC simulations specifically designed to avoid the previously reported shortcoming of the DG approach [7]. We compare the self-consistent simulations with results obtained using a ‘frozen field’ MC approximation and a ‘frozen quantum corrections’ approach.

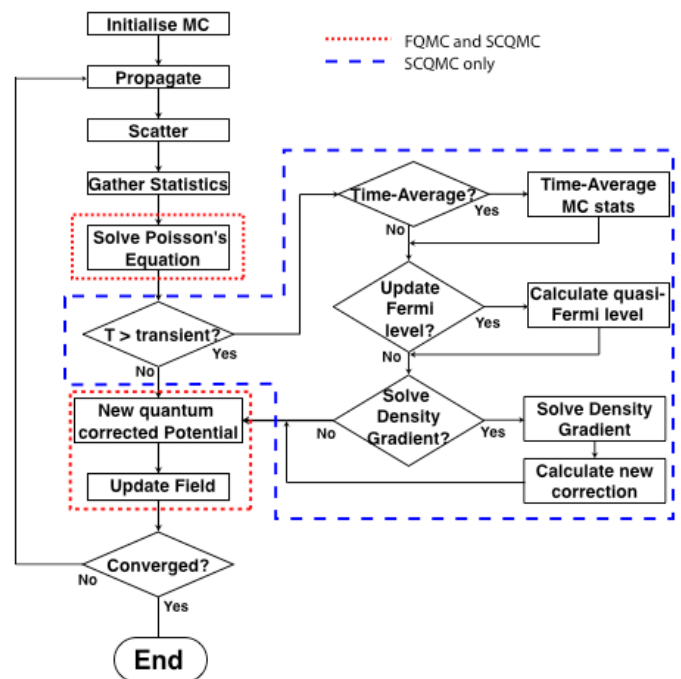


Figure 1. Flowchart showing the steps necessary for FFMC, FQMC and SCQMC simulations.

## II. SIMULATION METHODOLOGY

In the ‘frozen field’ approach (FFMC), used previously to study scattering from quantum confinement fluctuations in thin body devices [5], the quantum corrected potential is calculated from a DD simulation with Density Gradient quantum corrections, and is used in the MC module as the driving force for the particles, but is never updated.

The ‘frozen quantum corrections’ approach (FQMC) extracts the quantum correction term from initial DD simulations, but this time only the quantum corrections are stored and remain frozen, while the classical part of the potential is updated during the MC simulation via solution of Poisson’s equation based on the updated electron distribution after each time step. Hence, the driving force,  $F_q$ , is calculated using:

$$F_q = -\nabla(\psi_{cl} + \psi_{qc}) \quad (1)$$

Where  $\psi_{cl}$  is the classical potential and  $\psi_{qc}$  the stored correction term.

In the third, fully self-consistent, approach (SCQMC) the quantum correction is updated periodically throughout the course of the simulation. This is achieved by solving the density equation for electrons in respect of the electron concentration  $n_q$ :

$$\langle \phi_n \rangle_t - \langle \psi_{cl} \rangle_t + \frac{k_B T}{q} \ln \frac{n_q}{n_i} = 2b_n \frac{\nabla^2 \sqrt{n_q}}{\sqrt{n_q}} \quad (2)$$

Where  $\phi_n$  is the quasi Fermi level, and  $b_n = \hbar^2 / (12qm^*)$  and  $\langle \dots \rangle_t$  indicates a time-averaged value. A Maxwell-Boltzmann equation of state is assumed when deriving (2) [11]. Equation (2) is discretized using the finite box method, the corresponding system of equations is linearized and solved using a Red-Black SOR iterative scheme, which is easily amenable to parallelization. From the solution for  $n_q$ , which is reasonably smooth as a result of the averaging, a new value for  $\psi_{qc}$  is obtained using:

$$\psi_{qc} = \langle \phi_n \rangle_t + \frac{k_B T}{q} \ln \frac{n_q}{n_i} - \langle \psi_{cl} \rangle_t \quad (3)$$

The frequency of gathering statistics for time-averaging and for the solution of (2) remains subject to trial and error and requires further investigation perhaps being dependent on the architecture of the device in question, and the applied bias. Guide values ranging of 10 fs and 400 fs respectively have been successfully employed. As discussed in [12,13], the employment of Neumann boundary conditions at the source and drain end contacts when quantum corrections are employed in the simulations is necessary in order to prevent depletion in the contact regions that can lead to significant instabilities as the level of self-consistency increases.

The FFMC, FQMC and SCQMC methods are illustrated in the flowchart in Fig. 1, showing the additional steps needed as the level of self-consistency increases.

The test structure is a double gate (DG) MOSFET (illustrated in Fig. 2), with a 40 nm square channel and silicon body thickness of 2.4 nm. The oxide thickness is 1 nm and the doping is  $2 \times 10^{20} \text{ cm}^{-3}$  in the source and drain, and  $1 \times 10^{14} \text{ cm}^{-3}$  in the channel. Simulations at  $V_D = 1 \text{ mV}$  and 0.7 V have been carried out using DD and all three MC simulation methods. Fig. 3 compares the vertical potential obtained from DD, FQMC and SCQMC (gate to gate, as indicated in Fig. 2) at low  $V_D$  (where non-equilibrium effects are limited) showing an excellent agreement between the three simulation techniques. Also shown is the electron distribution through the same plane (this time including FFMC), which demonstrates an equally good match.

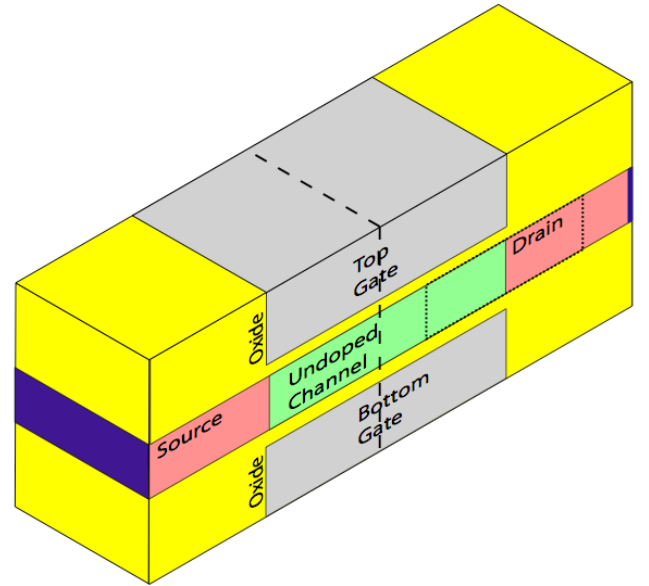


Figure 2. Schematic of the DG device used in this work, showing the plane through which Fig. 3 is taken (dashed line) and the region selected for Fig. 6 (dotted line).

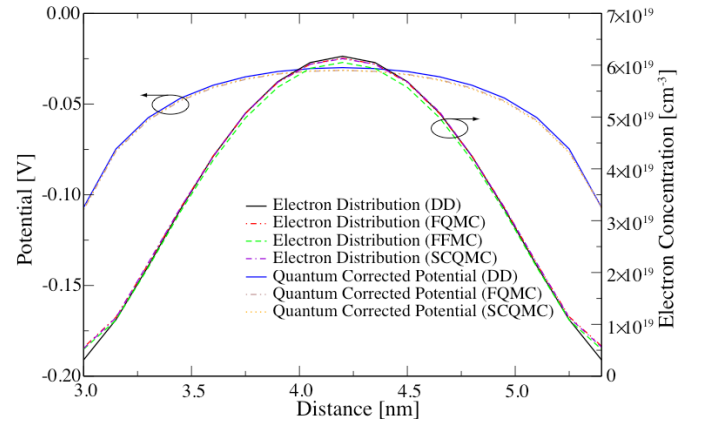


Figure 3. Vertical potential and electron distribution at  $V_D = 1 \text{ mV}$  from DD, FFMC (electron distribution only), FQMC and SCQMC showing good agreement.

### III. RESULTS AND DISCUSSION

Fig. 4 compares the  $I_D$ - $V_G$  characteristics at low and high  $V_D$  obtained using all simulation methodologies. At low  $V_D$  the DD simulations are calibrated by setting the low field mobility ( $\mu_0$ ) to that obtained at the source end of the channel (where  $I_D$  is determined [11]) in the equivalent FQMC simulation. At high  $V_D$ , a lateral field mobility model described by (4) is used with  $\mu_0$  calculated as before and the saturation velocity ( $v_{sat}$ ) set to the peak velocity obtained in the FQMC simulation, allowing for a good comparison between DD and MC.

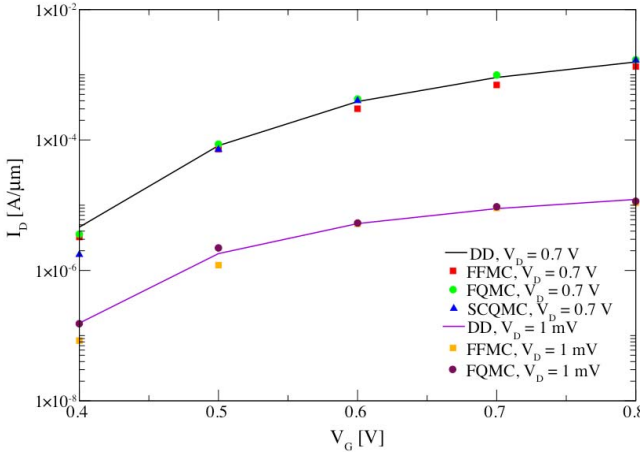


Figure 4.  $I_D$ - $V_G$  characteristics at  $V_D = 1$  mV and 0.7V from all simulators.

$$\mu = \frac{\mu_0}{\sqrt{1 + \frac{\mu_0 E_x^2}{v_{sat}^2}}} \quad (4)$$

Here, FFMC fails to accurately reproduce the value of  $I_D$  achieved by the other MC methods and the calibrated DD simulation. The explanation of this can be found in Fig. 5, which shows the velocity profiles from the MC simulations. The FFMC fails to account for the change of field moving from the source to the channel, hence the velocity adjusts much slower than the self-consistent MC simulations, giving an incorrect profile at the source end of the channel where  $I_D$  is determined [14]. Fig. 6 shows a comparison of the electron distribution in the silicon layer at  $V_D = 1$  mV from DD and FQMC showing an excellent agreement between the two.

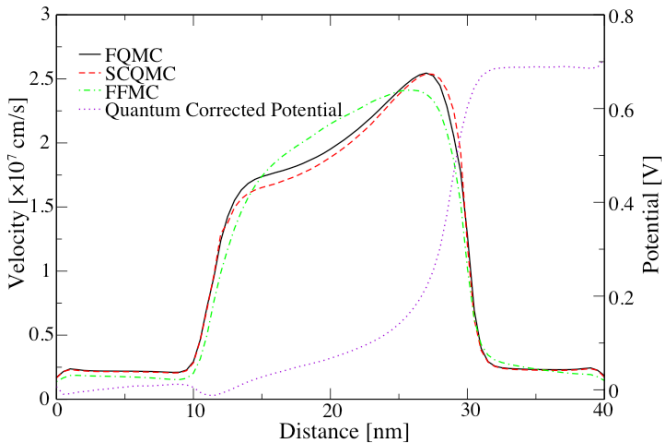


Figure 5. Velocity profiles at  $V_D = 0.7$  V for FFMC, FQMC and SCQMC and potential profile from FQMC.

Additionally, it can be noted that there is close agreement between the  $I_D$ - $V_G$  characteristics of FQMC and SCQMC, suggesting that frequent updating of the DG correction is unnecessary as the dynamic coupling between transport and field can be achieved via the solution to Poisson's equation alone, as with classical MC simulations. The correction, frozen or otherwise, accounts for the confinement effects, giving the correct shift of the electron concentration peak away from the oxide interface (as demonstrated in Fig. 3) along with the threshold voltage shift (as demonstrated in Fig. 7).

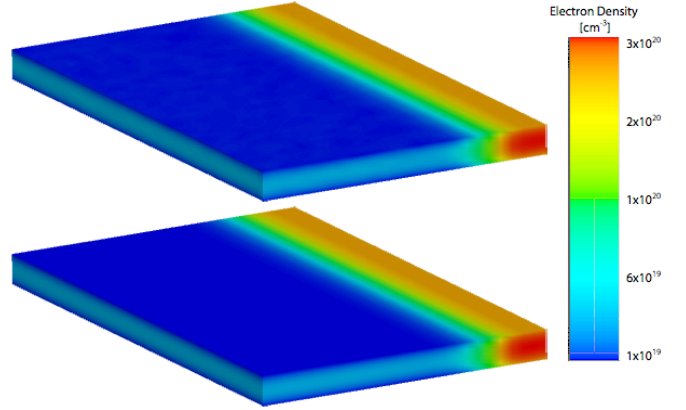


Figure 6. 3D view of the electron concentration in the drain end silicon layer (see Fig. 2) from DD (top) and FQMC (bottom) simulations at  $V_D = 1$  mV.

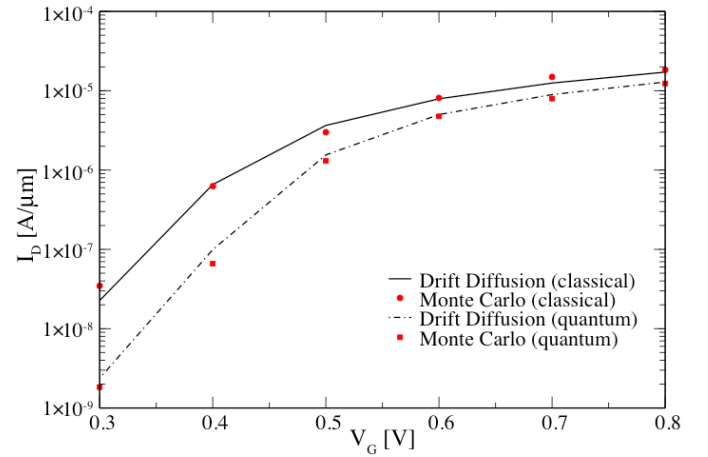


Figure 7.  $I_D$ - $V_G$  characteristics obtained using classical and quantum DD and FFMC simulations at  $V_D = 1$  mV demonstrating that the shift in  $V_T$  expected from the introduction of quantum corrections is captured by both methods. The device used in for this comparison was identical to that used in the course of this paper, except with a 50 nm square channel.

#### IV. CONCLUSIONS

We have presented a new methodology for incorporating Density Gradient quantum corrections into 3D MC simulations in a succession of increasingly self-consistent approaches. The fast, efficient FFMC approach has been expanded to FQMC and SCQMC approaches that add self-consistency with field and quantum correction respectively. We have been able to demonstrate the limitations of the FFMC as the applied drain voltage and the longitudinal field in the channel increases and transport becomes increasingly non-equilibrium, which this version of the methodology fails to accurately account for. The close agreement of FQMC and SCQMC suggests that self-consistency with the quantum correction term is not massively important, and that the introduction of quantum effects in this manner need only capture effectively the shifts in peak electron concentration and threshold voltage.

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