# A convergence enhancement method for deterministic multisubband device simulations of double gate PMOSFETs

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***Abstract*—For deterministic multisubband device simulations of double gate PMOSFETs, which are based on the self-consistent solution of Poisson-, $\vec{k}\cdot\vec{p}$ Schrödinger-, and Boltzmann transport equation, a new convergence enhancement method has been developed. The new approach is based on a Newton approach which considers the coupling between the Poisson equation and the Boltzmann transport equation. First order perturbation theory of the Schrödinger equation is employed for the calculation of the derivative of the Boltzmann transport equation w.r.t the electrostatic potential. The simulation results show that the new approach is efficient for both near-equilibrium and non-equilibrium situations.**

## I. Introduction

Multisubband device simulations for strained double gate PMOSFETs including magnetotransport have been published recently [1]. The Boltzmann transport equation (BTE) is solved by a deterministic (non Monte-Carlo) approach based on the Fourier expansion of the distribution function in the 2D $\vec{k}$-space [1], [2]. In [1] the system of the 1D $6\times 6$ $\vec{k}\cdot\vec{p}$ Schrödinger equation (SE), 2D Poisson equation (PE) and BTE within each subband is solved successively with a nonlinear relaxation scheme comparable to the classical Gummel loop until a self-consistent solution is obtained. This approach converges linearly with simulation time similar to the Gummel loops in the classical drift-diffusion based TCAD device simulators [3], [4], and thus much faster than a MC algorithm with its square root dependence [5]. In addition, it yields a truly stationary solution. Because the total CPU time is mainly dominated by the SE solver, it requires a new approach to reduce the number of Gummel type iteration steps.

## II. Convergence enhancement method

In this work, the convergence of the Gummel type iteration scheme in [1] is further enhanced by solving simultaneously the BTE and PE with a Newton approach. Self-consistency with the SE is again obtained by a Gummel type nonlinear relaxation scheme. The new approach converges faster than the previous nonlinear relaxation scheme because solving BTE and PE simultaneously by the Newton approach takes already care of the predominant part of the coupling between these equations.

The multisubband BTE does not depend explicitly on the electrostatic potential $V$ (solution of the PE). In order to capture most of the coupling between the BTE and PE the variation of the total subband energy appearing in the BTE is evaluated in terms of the variation of $V$ between Newton iteration steps $n$ and $n+1$ by applying first order perturbation theory to the $6\times 6$ $\vec{k}\cdot\vec{p}$ eigen problem. The variation of subband kinetic energy (structure of the 2D $\vec{k}$-space) is neglected and the variation of the total subband energy is further approximated such that it does not depend on the subband index. Using this approximation the derivative of the scattering integral w.r.t. $V$ vanishes. The derivative of the BTE w.r.t $V$ is therefore simple and involves only the drift term of the BTE. In the following the details of the method are described.

The coupled system of PE and BTE which is intended to be solved by a Newton-Raphson iteration scheme is written as:

$$F_{\mathrm{PE}}(V(x,z),g_m^\nu(x,\tilde{\varepsilon})) = 0 \quad (1)$$

$$F_{\mathrm{BTE}}(V(x,z),g_m^\nu(x,\tilde{\varepsilon})) = 0 \quad (2)$$

where $x,z$ are the positions along the transport and quantization directions, respectively. Here $\tilde{\varepsilon}$ is the kinetic subband energy, $V$ the electrostatic potential, and $g_m^\nu$ the Fourier expansion coefficient of order $m$ for the generalized distribution function belonging to subband $\nu$.

For the Newton-Raphson iteration step $(n+1)$, the $V$ and $g_m^\nu$ corrections, denoted as $\delta V$ and $\delta g_m^\nu$, are the solution of the coupled system of equations:

$$-F_{\mathrm{PE}}^{(n)} = \frac{\partial F_{\mathrm{PE}}}{\partial V(x,z)}\delta V(x,z)+\frac{\partial F_{\mathrm{PE}}}{\partial g_m^\nu(x,\tilde{\varepsilon})}\delta g_m^\nu(x,\tilde{\varepsilon}) \quad (3)$$

$$-F_{\mathrm{BTE}}^{(n)} = \frac{\partial F_{\mathrm{BTE}}}{\partial V(x,z)}\delta V(x,z)+\frac{\partial F_{\mathrm{BTE}}}{\partial g_m^\nu(x,\tilde{\varepsilon})}\delta g_m^\nu(x,\tilde{\varepsilon}) \quad (4)$$

using a Taylor series expansion of (1) and (2) up to first order.

As soon as the solutions $\delta V$ and $\delta g_m^\nu$ are available, the unknowns of the system (1) and (2) can be updated:

$$V^{(n+1)}(x,z) = V^{(n)}(x,z)+\delta V(x,z) \quad (5)$$

$$g_m^{\nu(n+1)}(x,\tilde{\varepsilon}) = g_m^{\nu(n)}(x,\tilde{\varepsilon})+\delta g_m^\nu(x,\tilde{\varepsilon}) \quad (6)$$

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With the updated $V$ and $g_m^\nu$, the correction procedure is repeated for the next iteration step. The iteration converges when the corrections $|\delta V|$ and $|\delta g_m^\nu|$ get smaller than a preset criterion.

Except $\frac{\partial F_{\text{BTE}}}{\partial V(x,z)}$, the derivatives appearing in (3) and (4) can be calculated in a straightforward manner. A direct calculation of $\frac{\partial F_{\text{BTE}}}{\partial V(x,z)}$ is impossible because the multisubband BTE does not depend explicitly on $V$. Actually the electrostatic potential $V$ entering the $6 \times 6$ $\vec{k} \cdot \vec{p}$ Schrödinger eigen problem is captured by the multisubband BTE implicitly through the total subband energy, which is the eigen energy of the eigen problem. In order to obtain an explicit coupling between BTE and PE, the variation of the total subband energy $\delta\varepsilon^\nu(x,\vec{k}) \equiv \varepsilon^{\nu,(n+1)}(x,\vec{k}) - \varepsilon^{\nu,(n)}(x,\vec{k})$ is evaluated in terms of the variation of the electrostatic potential $\delta V(x,z)$ using first order perturbation theory (here $\vec{k}$ is the wave vector in the 2D $\vec{k}$-space).

The perturbed Hamiltonian is given by the variation of the electrostatic potential, and the variation of the eigen energy between iteration $n+1$ and $n$ can be determined by first order perturbation theory:

$$\begin{aligned} \delta\varepsilon^\nu(x,\vec{k}) &= \int \vec{\zeta}^{\nu\dagger}(x,z,\vec{k})\delta V(x,z)\vec{\zeta}^{\nu}(x,z,\vec{k})dz \\ &= \int \mathcal{P}^\nu(x,z,\vec{k})\delta V(x,z)dz \end{aligned} \tag{7}$$

The wave function $\vec{\zeta}$ (the eigen vector of the eigen problem) is assumed to be unchanged during the Newton-Raphson iteration process. Consequently the probability density function $\mathcal{P} = \vec{\zeta}^\dagger\vec{\zeta}$ is the same for all Newton-Raphson iteration steps.

In order to simplify the derivative w.r.t $V$ of the scattering integral of the multisubband BTE, $\delta\varepsilon^\nu(x,\vec{k})$ is further approximated so that it does not depend on the subband index or wave vector. Multiplying the aforementioned $\delta\varepsilon^\nu(x,\vec{k})$ with the distribution function $f^{\nu,(n)}(x,\vec{k})$ and then integrating over $\vec{k}$-space and summing over all subband indices gives:

$$\begin{aligned} &\sum_\nu \frac{1}{(2\pi)^2}\int \delta\varepsilon^\nu(x,\vec{k})f^{\nu,(n)}(x,\vec{k})d^2k \\ &= \sum_\nu \frac{1}{(2\pi)^2}\int\int \mathcal{P}^\nu(x,z,\vec{k})\delta V(x,z)dz f^{\nu,(n)}(x,\vec{k})d^2k \\ &= \int \delta V(x,z)p^{(n)}(x,z)dz \end{aligned} \tag{8}$$

where $p^{(n)}(x,z)$ is the hole density after iteration step $n$ given by:

$$p^{(n)}(x,z) = \sum_\nu \frac{1}{(2\pi)^2}\int \mathcal{P}^\nu(x,z,\vec{k})f^{\nu,(n)}(x,\vec{k})d^2k \tag{9}$$

The total subband energy is decomposed into a potential subband energy $\varepsilon_{\text{pot}}$ and a kinetic subband energy $\tilde{\varepsilon}$ as follows [6]:

$$\varepsilon^\nu(x,\vec{k}) = \varepsilon^\nu_{\text{pot}}(x) + \tilde{\varepsilon}^\nu(x,\vec{k}) \tag{10}$$

fulfilling $\tilde{\varepsilon}^\nu(x,\vec{k}=\vec{0}) = 0$ for all position $x$ along the transport direction. If the total subband energy variation is assumed to be dominated by the variation of the subband potential energy $\delta\varepsilon^\nu_{\text{pot}}(x)$, which in turn is assumed to be the same for all subbands:

$$\delta\tilde{\varepsilon}^\nu(x,\vec{k}) \approx 0 \tag{11}$$

$$\delta\varepsilon^\nu_{\text{pot}}(x) \approx \delta\varepsilon_{\text{pot}}(x) \tag{12}$$

then the LHS of (8) can be simplified:

$$\begin{aligned} &\sum_\nu \frac{1}{(2\pi)^2}\int \delta\varepsilon^\nu(x,\vec{k})f^{\nu,(n)}(x,\vec{k})d^2k \\ &\approx \delta\varepsilon_{\text{pot}}(x)\sum_\nu \frac{1}{(2\pi)^2}\int f^{\nu,(n)}(x,\vec{k})d^2k \\ &= \delta\varepsilon_{\text{pot}}(x)\int p^{(n)}(x,z)dz \end{aligned} \tag{13}$$

The final equality in (13) is obtained directly from (9) with $\int \mathcal{P}^\nu(x,z,\vec{k})dz = 1$.

Thus the variation of the potential energy, which does not depend on the subband index, is obtained:

$$\delta\varepsilon_{\text{pot}}(x) = \frac{\int \delta V(x,z)p^{(n)}(x,z)dz}{\int p^{(n)}(x,z)dz} \tag{14}$$

With (11) and (14) the derivative w.r.t $V$ of the drift operator (LHS of multisubband BTE) can be evaluated. Moreover, the derivative of the drift operator using (11) and (14) is much simpler than the calculation based on (7), which depends on the subband index and wave vector.

The derivative w.r.t $V$ of the scattering integral (the RHS of multisubband BTE) involves only the derivative w.r.t $V$ of the kinetic subband energy of the initial and final states in Fermi's Golden Rule [7], [8]:

$$\tilde{\varepsilon}^{\nu'}(x,\vec{k}') + \varepsilon^{\nu'}_{\text{pot}}(x) = \tilde{\varepsilon}^\nu(x,\vec{k}) + \varepsilon^\nu_{\text{pot}}(x) \mp \Delta\varepsilon_{\text{trans.}} \tag{15}$$

Here $\Delta\varepsilon_{\text{trans.}}$ is the transfer energy due to scattering (e.g. optical phonon energy). The variations of the initial and final energies cancel each other

$$\delta\varepsilon^\nu_{\text{pot}}(x) = \delta\varepsilon^{\nu'}_{\text{pot}}(x) \tag{16}$$

in the energy conserving delta function of Fermi's Golden Rule due to approximation (12). Therefore the derivative of the scattering integral w.r.t $V$ vanishes.

## III. Results

A 16nm gate length Si double gate PMOSFET is simulated. The Si body and oxide thicknesses of the double gate structure are 5nm and 0.7nm, respectively. (001) wafer surface and [110] channel orientation are considered. Scattering due to phonons and surface roughness is included. More details about the scattering model can be found in [9], [2]. A constant lattice temperature of 300K is assumed. The work function was chosen such that the threshold voltage is about 0.18V. The simulations are preformed for both near- and none-equilibrium transport.

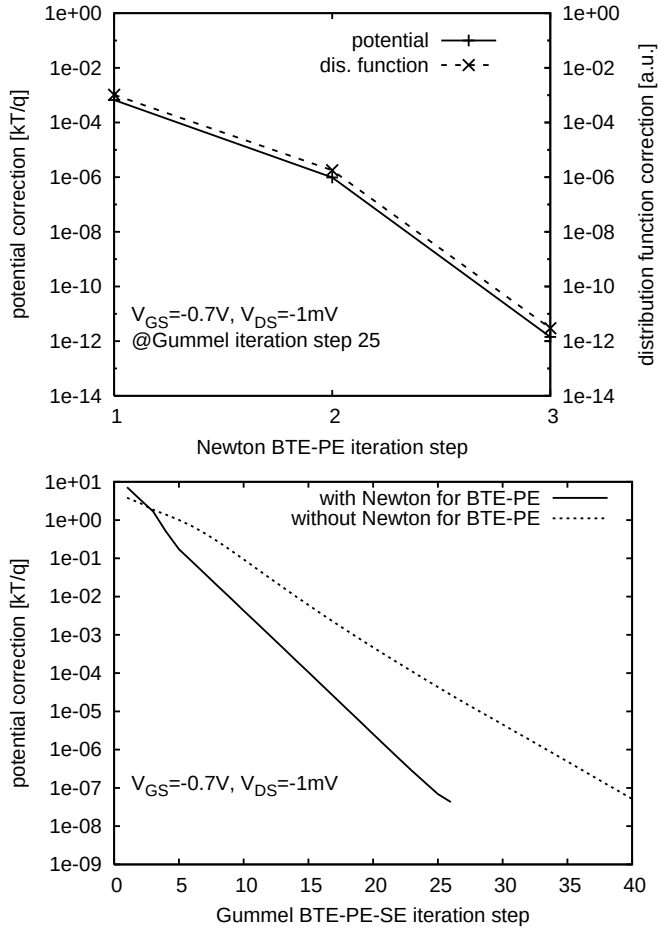


Fig. 1. Convergence of BTE-PE Newton method (top) and of the BTE-PE-SE Gummel loops (bottom). $V_{GS} = -0.7$V, $V_{DS} = -1$mV.

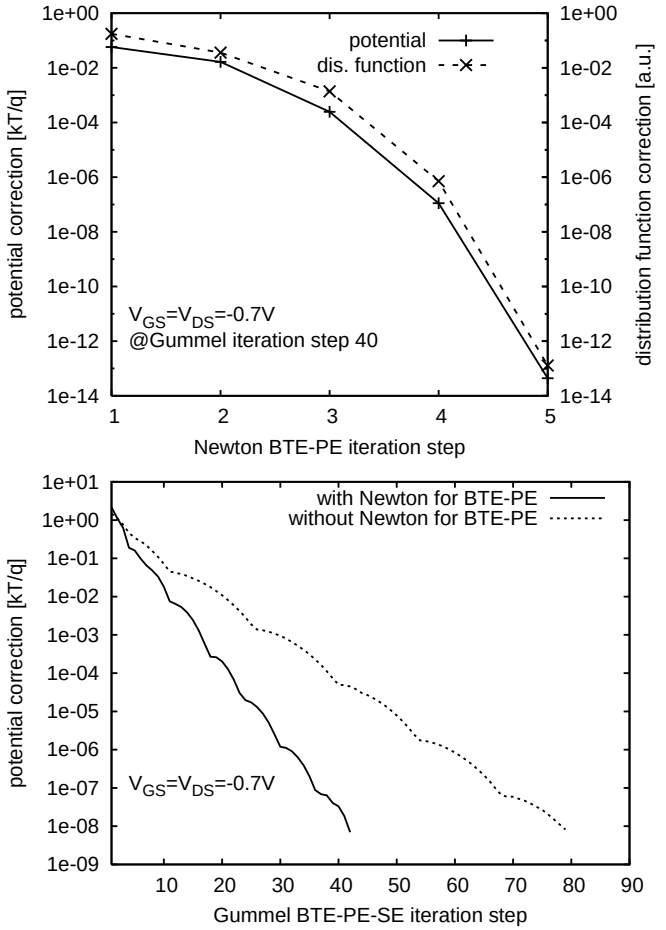


Fig. 3. Convergence of the BTE-PE Newton method (top) and of the BTE-PE-SE Gummel loops (bottom). $V_{GS} = V_{DS} = -0.7$V.

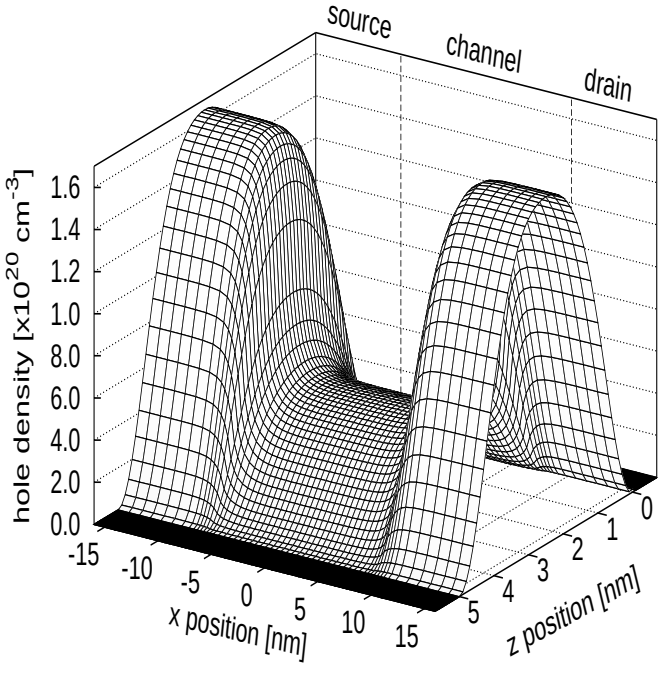


Fig. 2. Self-consistent hole density within the device. $x$ is the transport direction and $z$ is the quantization direction. $V_{GS} = -0.7$V, $V_{DS} = -1$mV.

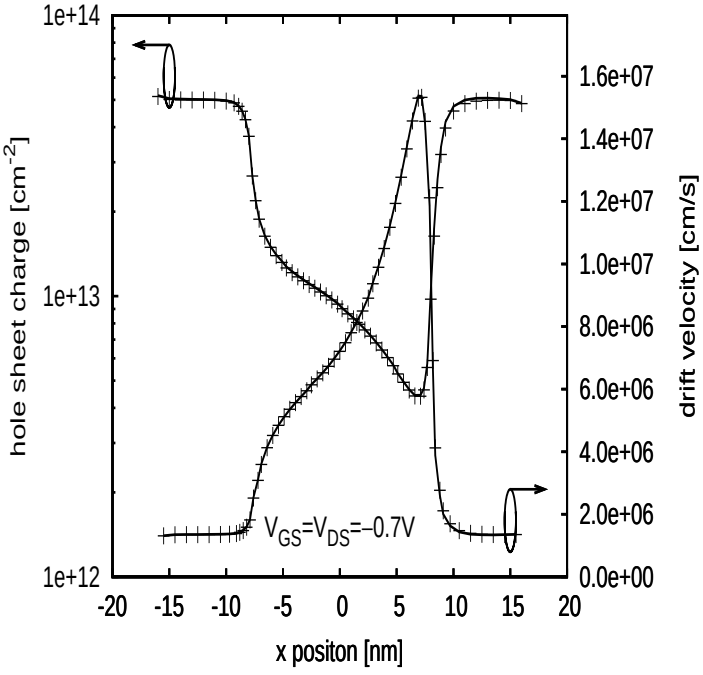


Fig. 4. Self-consistent solution of the hole sheet charge and the drift velocity along the transport direction $x$. $V_{GS} = V_{DS} = -0.7$V.

For $V_{GS} = -0.7$V and $V_{DS} = -1$mV (near equilibrium), the convergence of the Newton approach for the BTE-PE subsystem and the convergence of the outer Gummel type loops for the BTE-PE-SE system are shown in Fig. 1. The typical quadratic convergence of a Newton approach is visible in Fig. 1 (top). Fig. 1 (bottom) shows clearly that the introduction of the Newton approach improves the convergence speed of the nonlinear relaxation loops very much. In order to achieve an electrostatic potential correction of $10^{-7}kT/q$, the new approach requires only 24 Gummel type iteration steps instead of 39 needed by the old relaxation method. The CPU time per iteration, which is dominated by the SE solver, is nearly the same for the old and the new nonlinear relaxation scheme. The hole density (Fig. 2) within the device evaluated by the self-consistent solution of the BTE-PE-SE system clearly shows that the size quantization is considered not only for the channel region but also for the source and drain regions.

Similar to Fig. 1, Fig. 3 again shows the convergence of the Newton method and the convergence of the outer Gummel type loops with and without the new Newton step for a high drain bias typically used for $I_{ON}$ calculations. The quadratic behavior of potential and distribution function corrections during the Newton process is again observable. Moreover the enormous convergence enhancement of the nonlinear relaxation scheme due to the new approach is again observable for this strong non-equilibrium condition. Self-consistent solutions for the hole sheet charge and the drift velocity along the channel are shown in Fig. 4.

## IV. Conclusion

A new convergence enhancement method for deterministic multisubband device simulations has been developed. The new approach is based on a Newton approach which considers for the first time the coupling between the PE and the BTE introduced by the subband structure within a realistic device in a highly efficient manner. The new method reduces the number of Gummel type iteration steps and consequently the CPU time for achieving a self-consistent solution of high accuracy by about a factor of 2. The new approach is efficient for both near-equilibrium and non-equilibrium situations.

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