A Fast, Numerical Circuit-Level Model of Carbon Nanotube Transistor

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Abstract

Recently proposed circuit-level models of carbon nanotube transistor (CNT) for SPICE-like simulators suffer from numerical complexities as they rely on numerical evaluation of integrals or internal Newton-Raphson iterations to find solutions of non-linear dependencies or both. Recently an approach has been proposed which eliminates the need for numerical integration when calculating the charge densities in CNTFET through the use of piece-wise linear approximation. This paper builds on the effective employment of linear approximation to accelerate the CNT model speed when evaluating the source-drain current of the CNT, but rather than using symbolic solutions as reported, we propose to employ a numerical linearization of charge density dependence on the self-consistent voltage to obtain a dramatic reduction in the CPU time. Our results show a speed up of up to almost four orders of magnitude compared with the theoretical CNT model implemented in FETToy, used as a reference for verifying newer models. Comparisons of drain-source current characteristics of the new model against that in FETToy are presented, confirming the accuracy of the proposed approach.

1. Introduction

While it is gradually becoming more clear how the Carbon Nanotube Transistor (CNT) operates [1, 2], several SPICE-compatible models have recently been proposed (eg. [3, 4, 5, 6, 7, 8]) in anticipation that analog and digital systems built with CNT devices will soon need to be simulated at the circuit level. Most proposed models rely on an estimation of the mobile charge densities from which the total drain current is derived [1]. Accurate calculation of the mobile charge involves integrating the densities of states over the number of allowed energy levels using the Fermi probability distribution. As the total drain-source current is driven by the self-consistent voltage, which comprises i.a. the drain-source bias voltage as well as potential induced by the non-equilibrium mobile charge injected from the source and drain, a solution of non-linear algebraic equations is necessary to calculate the drain current. Numerical evaluations of integrals and iterative solutions of non-linear algebraic equations (usually by the Newton-Raphson approach) are time consuming and may be impractical in simulations involving large numbers of CNT devices of varying parameters. The well known MATLAB script named FETToy [9] requires more than 12 seconds of the CPU time on a Pentium IV based PC to calculate a family of CNT current drain characteristics. A recent interesting approach [8] proposes a piece-wise linear approximation of the charge density profiles to simplify calculations. In this contribution we further simplify and generalize the charge density linearization and obtain a speed-up of approximately 8000 times, which represents almost four orders of magnitude, compared with FETToy. As our results demonstrate, the loss of accuracy due to charge density linearization is insignificant.

2. Fast circuit-level CNT model

When a voltage $V_{DS} > 0$ is applied to the drain and source of a top-gate or a bottom-gate CNT [10, 11] the following non-equilibrium mobile charge density is induced [1]

$$\Delta Q = q(N_S + N_D - N_0)$$  \hspace{1cm} (1)

where $N_S$ is the density of positive velocity states filled by the source, $N_D$ is the density of negative velocity states filled by the drain and $N_0$ is the equilibrium electron density. These densities are given by

$$N_S = \frac{1}{2} \int_{-\infty}^{+\infty} D(E) f(E - U_{SF}) dE$$  \hspace{1cm} (2)

$$N_D = \frac{1}{2} \int_{-\infty}^{+\infty} D(E) f(E - U_{DF}) dE$$  \hspace{1cm} (3)
\[ N_0 = \int_{-\infty}^{+\infty} D(E) f(E - E_F) dE \] (4)

where \( U_{SF} \) and \( U_{DF} \) are defined as

\[ U_{SF} = E_F - qV_{SC} \] (5)

\[ U_{DF} = E_F - qV_{SC} - qV_{DS} \] (6)

\( V_{SC} \) is the self-consistent voltage, \( D(E) \) is the density of states, \( E_F \) is the Fermi level, \( f \) is the Fermi probability distribution, \( q \) is the electronic charge and \( E \) represents the energy levels per CNT unit length.

The self-consistent voltage \( V_{SC} \) is derived from the total device charge density and hence must be calculated using an implicit relationship. This relationship is given by the following equation [8]

\[ V_{SC} = -\frac{Q_t + qN_S(V_{SC}) + qN_d(V_{SC}) + qN_0}{C_\Sigma} \] (7)

where \( Q_t \) represents the charge stored in terminal capacitances and is defined as

\[ Q_t = V_GC_G + V_DC_D + V_SC_S \] (8)

where \( C_G, C_D, C_S \) are the gate, drain, and source capacitances correspondingly and the total terminal capacitance \( C_\Sigma \) is

\[ C_\Sigma = C_G + C_D + C_S \] (9)

For the purpose of circuit modeling, we propose to apportion equal parts of the equilibrium mobile charge density \( N_0 \) to the drain and source, and introduce the corresponding non-equilibrium mobile charge densities \( Q_S \) and \( Q_D \) as follows

\[ Q_S(V_{SC}) = q(N_S - \frac{1}{2}N_0) \] (10)

and

\[ Q_D(V_{SC}) = q(N_D - \frac{1}{2}N_0) \] (11)

The non-equilibrium mobile charges can now be represented as circuit capacitances as shown in the equivalent circuit of the model in figure 1 connected between the drain and source correspondingly and the inner node \( \Sigma \) that represents a hypothetical point which combines all the CNT charges that affect the self-consistent voltage and hence the drain-source current \( I_{DS} \). As in our model the self-consistent voltage \( V_{SC} \) is a piece-wise linear function of the terminal voltages \( V_G, V_S \) and \( V_D \), the capacitances which

store the source and drain mobile charges \( Q_S \) and \( Q_D \) are also piece-wise linear and controlled by the terminal voltages.

As it has already been highlighted in Introduction above, evaluation of the self-consistent voltage directly from equation (7) involves a time consuming Newton-Raphson iterative process. Each Newton-Raphson iteration in turn requires evaluations of integrals to obtain state densities \( N_s(V_{SC}) \) and \( N_d(V_{SC}) \). Below we show how these calculations can be vastly simplified without a significant loss of accuracy. The typical dependence of non-equilibrium mobile charge density at the source, calculated from equations (3) and (10), is illustrated in figure 2. Corresponding graphs for the drain charge density have similar shapes. Figure 2 also shows sample piece-wise linear approximations of the charge density curves. As explained below, this numerical linearization, where piece-wise linear regions are expressed by equations (15) and (16), leads to vast CPU time savings as it completely eliminates the need for Newton-Raphson iterations and numerical evaluation of state density integrals.

Unlike what has been proposed in a recent publication [8], that a three-piece linear approximation of the state densities should rely on symbolic calculations of slopes and intersection points from CNT parameters, the approach we suggest here is to not to link the slopes and intersection points to CNT parameters directly but rather to use an arbitrary number of them and adjust their slopes and intersection points to maximize the overall drain current characteristic accuracy. In the next section we show test results with this approach applied to a 3-range and 5-range piece-wise linear approximation of the charge densities. This, purely numerical rather than symbolic, approach not only gives the model developer more control over the accuracy but also leads to a dramatic saving in the processing time.
CNT transport theory [1, 9] as follows

The CPU time is reduced by up to almost four orders of magnitude compared with the theoretical model [1] implemented in FETToy [9], as demonstrated in section 3.

The drain current can be approximated from the ballistic approximation.

Figure 2. Charge density dependence on self-consistent voltage for $E_f=0$, -0.32 and -0.5 eV. Dashed lines represent a sample linearized approximation.

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The model presented in the previous section has a form suitable for a direct implementation in a SPICE-like simulator. SPICE and most other analog and mixed-signal circuit simulators formulate their analog system equation set from companion models which contain derivatives of model equations with regards to the unknown variables. Partial derivatives of \( I_{DS} \) with regard to the terminal voltages \( V_G, V_S \) and \( V_D \) can be obtained in analytical form as follows

\[
\frac{\partial I_{DS}}{\partial V_G} = \frac{\partial I_{DS}}{\partial U_{SF}} \frac{\partial U_{SF}}{\partial V_G} + \frac{\partial I_{DS}}{\partial U_{DF}} \frac{\partial U_{DF}}{\partial V_G}
\]  (18)
\begin{align}
\frac{\partial I_{DS}}{\partial V} &= \frac{\partial I_{DS}}{\partial U_{SF}} \frac{\partial U_{SF}}{\partial V} + \frac{\partial I_{DS}}{\partial U_{DF}} \frac{\partial U_{DF}}{\partial V} 
\tag{19} \\
\frac{\partial I_{DS}}{\partial V_D} &= \frac{\partial I_{DS}}{\partial U_{SF}} \frac{\partial U_{SF}}{\partial V_D} + \frac{\partial I_{DS}}{\partial U_{DF}} \frac{\partial U_{DF}}{\partial V_D} 
\tag{20}
\end{align}

Equations (5) and (6) yield

\begin{align}
\frac{\partial U_{SF}}{\partial V_G} &= \frac{\partial U_{DF}}{\partial V_G} = -q \frac{\partial V_{SC}}{\partial V_G} 
\tag{21} \\
\frac{\partial U_{SF}}{\partial V_S} &= -q \frac{\partial V_{SC}}{\partial V_S} 
\tag{22} \\
\frac{\partial U_{SF}}{\partial V_S} &= -q \frac{\partial V_{SC}}{\partial V_S} 
\tag{23} \\
\frac{\partial U_{DF}}{\partial V_S} &= -q \left( 1 + q \frac{\partial V_{SC}}{\partial V_S} \right) 
\tag{24} \\
\frac{\partial U_{DF}}{\partial V_D} &= -q \left( 1 + q \frac{\partial V_{SC}}{\partial V_D} \right) 
\tag{25}
\end{align}

From equation (7) and the linearised approximation defined by equations (15) and (16), $V_{SC}$ derivatives are constant in each piece-wise region and can be estimated as:

\begin{align}
\frac{\partial V_{SC}}{\partial V_G} &= \frac{C_G}{C_S + q(A_s + A_d)} 
\tag{26} \\
\frac{\partial V_{SC}}{\partial V_S} &= \frac{C_S}{C_S + q(A_s + A_d)} 
\tag{27} \\
\frac{\partial V_{SC}}{\partial V_D} &= \frac{C_S}{C_S + q(A_s + A_d)} 
\tag{28}
\end{align}

Hence, from the above equations, equation (12) and equation (14), the drain current derivatives required to create a companion model for an analog circuit solver can be estimated as

\begin{align}
\frac{\partial I_{DS}}{\partial V_G} &= qI_0 \frac{C_G}{kT C_T} \left( \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} - \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} \right) 
\tag{29} \\
\frac{\partial I_{DS}}{\partial V_S} &= \frac{qI_0 C_S}{kT C_T} \left( \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} - \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} \right) + \frac{qI_0}{kT} \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} 
\tag{30} \\
\frac{\partial I_{DS}}{\partial V_D} &= \frac{qI_0 C_D}{kT C_T} \left( \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} - \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} \right) + \frac{qI_0}{kT} \frac{1}{1 + e^{\frac{U_{DF}}{kT}}} 
\tag{31} \end{align}
5. Conclusion

We have proposed a new, fast numerical CNT model suitable for a direct implementation in SPICE-like simulators. Results provide further evidence to support the recent suggestion [8] to avoid the use of numerical integration when calculating charge densities in the CNT model, leading to significant speed up in the model simulation. We have proposed to apply an arbitrary number of linear approximation regions to the non-equilibrium mobile charge densities rather than the symbolic three-piece form [8]. The mobile charge densities are represented in a form suitable for a direct implementation in a circuit model. When compared with FETToy [9], a reference theoretical CNT model, we have demonstrated that the proposed approximation approach leads to a dramatic computational cost saving without sacrificing the modeling accuracy. Findings of this research contribute towards the current efforts in nanoelectronic circuit design that include development of fast and accurate CNFET models with the aim to enable circuits with large numbers of such devices to be simulated efficiently and accurately. Future work will involve development of automated optimization techniques for the mobile charge density piece-wise linear approximations such that the $I_{DS}$ prediction accuracy can be further increased while maintaining the fast execution speed.

References


