Abstract—This paper presents the algorithms of an implementation of a numerically efficient carbon nanotube transistor (CNT) model in HSPICE. The model is derived from cubic spline non-linear approximation of the non-equilibrium mobile charge density. The spline algorithm exploits a rapid and accurate solution of the numerical relationship between the charge density and the self-consistent voltage, which results in the acceleration of deriving the current through the channel without losing much accuracy. The output I-V characteristics of the proposed model have been compared with those of a recent HSPICE implementation of the Stanford CNT model and published experimental I-V curves. The results show superior accuracy of the proposed model while maintaining similar CPU time performance. Two versions of the HSPICE macromodel implementation have been developed and validated, one to reflect ballistic transport only and another with non-ballistic effects. To further validate the model a complementary logic inverter has also been implemented using the proposed technique and simulated in HSPICE.

I. INTRODUCTION

Transistors using carbon nanotubes (CNTs) have shown the potential of becoming the basis of next generation integrated circuits (ICs) [1], [2]. A number of theoretical models have been proposed to describe the different physical phenomena within the nanotube channel and their effect on the performance of the device [3], [4], [5], [6], [7], [8]. The standard modelling methodology relies on repetitive numerical evaluation of the Fermi-Dirac integral to obtain the drain-source current for a given set of terminal potential. Recently improved approaches have been proposed where the slow iterative process is replaced by direct calculations using numerically efficient approximations while still maintaining good accuracy compared with the basic theory [6], [9]. These new techniques rely on piece-wise approximation of charge densities, either linear [6] or non-linear [9] to simplify the numerical calculation. The improved models have been implemented and tested in MATLAB and VHDL-AMS [10]. Here we propose a more practical implementation using the HSPICE macromodelling language [11]. The model has been validated using sample transistor circuits and logic gates and demonstrated to compare favourably in terms of accuracy with the recently released Stanford HSPICE CNT model. The HSPICE model proposed here has been demonstrated to have the potential of including non-ballistic effects in the evaluation of the drain current.

II. CALCULATION OF THE SELF-CONSISTENT VOLTAGE

When voltages are applied to the drain and the source of a CNT transistor as illustrated in figure 1, a non-equilibrium mobile charge is generated in the carbon nanotube channel, which can be described in as follows[1], [12], [13]:

\[ \Delta Q = q(N_S + N_D - N_0) \]  

(1)

where \( N_S \) is the density 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 determined by the Fermi-Dirac probability distribution:

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

(2)

\[ N_D = \frac{1}{2} \int_{-\infty}^{+\infty} D(E) f(E - U_{DF}) dE \]  

(3)

\[ N_0 = \int_{-\infty}^{+\infty} D(E) f(E - E_F) dE \]  

(4)

where \( D(E) \) is the density of states, \( f \) is the Fermi probability distribution, \( E \) represents the energy levels per nanotube unit length, and \( U_{SF} \) and \( U_{DF} \) are introduced as

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

(5)

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

(6)

where \( E_F \) is the Fermi level, \( q \) is the electronic charge and \( V_{SC} \) represents the self-consistent voltage [1] whose presence in these equations illustrates that the CNT energy band is affected by external terminal voltages. The self-consistent
voltage $V_{SC}$ is determined by the device terminal voltages and charges at terminal capacitances by the following non-linear algebraic equation [1], [6]:

$$V_{SC} = -\frac{Q_i + qN_S(V_{SC}) + qN_D(V_{SC}) + qN_t}{C_\Sigma}$$  \hspace{1cm} (7)

where $Q_i$ represents the charge stored in terminal capacitances and is defined as

$$Q_i = V_G C_G + V_D C_D + V_S C_S + V_{Sub} C_{Sub}$$  \hspace{1cm} (8)

where $C_G, C_D, C_S, C_{Sub}$ are the gate, drain, source and substrate capacitances correspondingly and the total terminal capacitance $C_\Sigma$ is

$$C_\Sigma = C_G + C_D + C_S + C_{Sub}$$  \hspace{1cm} (9)

$$C_{ox} = 2\pi k_1 \varepsilon_0 / \ln(2t_{ox} + d)$$  \hspace{1cm} (10)

$$C_{Sub} = 2\pi k_2 \varepsilon_0 / \ln(4H_{Sub}/d)$$  \hspace{1cm} (11)

where $d$ is the diameter of the carbon nanotube, $H_{Sub}$ is the thickness of the $SiO_2$ layer on the substrate, $t_{ox}$ is the thickness of the gate insulator and $k_1$, $k_2$ are the relative permittivities of the gate and the substrate respectively [14]. Meanwhile, the capacitances between terminals can be obtained as follows as reported previously [15].

$$C_G = C_{ox}$$  \hspace{1cm} (12)

$$C_S = 0.097C_{ox}$$  \hspace{1cm} (13)

$$C_D = 0.040C_{ox}$$  \hspace{1cm} (14)

According to the ballistic CNT ballistic transport theory [1], [15] the drain current caused by the transport of the non-equilibrium charge across the nanotube can be calculated using the Fermi-Dirac statistics as follows:

$$I_{DS0} = \frac{2qkT}{\pi \hbar} \left[ \mathcal{F}_0 \left( \frac{U_{SF}}{kT} \right) - \mathcal{F}_0 \left( \frac{U_{DF}}{kT} \right) \right]$$  \hspace{1cm} (15)

where $\mathcal{F}_0$ represents the Fermi-Dirac integral of order 0, $k$ is Boltzmann’s constant, $T$ is the temperature and $\hbar$ is reduced Planck’s constant.

The numerical efficiency of the ballistic CNT transport model presented above hinges on an efficient calculation of the non-equilibrium mobile charge. Piecewise approximation of the mobile charge based on cubic splines significantly accelerates calculations without losing much accuracy [9]. The mobile charge can be presented as a function of a single variable, the self-consistent voltage $V_{SC}$:

$$Q(V_{SC}) = \frac{q}{2} \int_{-\infty}^{+\infty} D(E) f(E - E_F - V_{SC}) dE$$  \hspace{1cm} (16)

Hence, a simple spline structure, using $n$ equally spaced points, can easily be constructed to approximate the mobile charge dependence on $V_{SC}$. If cubic splines are used, the individual polynomial pieces have the following form

$$Q(V_{SC}) = a_i V_{SC}^3 + b_i V_{SC}^2 + c_i V_{SC} + d_i$$  \hspace{1cm} (17)

where $a_i$, $b_i$, $c_i$ and $d_i$, $i = 1, \ldots, n - 1$ are spline coefficients. This enables a closed-form solution of the self-consistent voltage equation (7) as, for each piece, it now becomes a polynomial equation of the third order. Thus, the need for costly Newton-Raphson iterations and evaluations of Fermi-Dirac integrals is eliminated. Once the self-consistent voltage $V_{SC}$ is efficiently calculated from the closed-form solutions of equation (7), the total drain current can be directly obtained from equations (5), (6) and (15).

Figure 2 shows $I_{DS}$ characteristics obtained from a MATLAB simulation, where an example model that uses three cubic splines, $n = 4$, and two linear pieces at the ends was compared with the theoretical curves calculated by FETToy from equations (3) and (4) correspondingly.

![Figure 2](image)

**Fig. 2.** Drain current characteristics at $T = 300K$ and $E_F = -0.32eV$ for FETToy(solid lines) and 3 pieces cubic spline approximation (dashed lines).

To solve the resulting 3rd order polynomial equations, Cardano’s method [16] is applied to determine the appropriate root which represents the correct value of $V_{SC}$. Since the self-consistent voltage $V_{SC}$ is directly obtained from the spline model, the evaluation of the drain current poses no numerical difficulty as energy levels $U_{SF}$, $U_{DF}$ can be found quickly from equations (5), (6) and $I_{DS}$ can be calculated using equation (15).

**III. HSPICE MACROMODEL IMPLEMENTATION**

Having implemented the spline-based numerical model in MATLAB, HSPICE macromodels of an n-type-like and p-type-like CNT transistor have been developed. Figure 3 shows
the \( I_{DS} \) characteristics of the n-type-like transistor implemented in HSPICE compared with the output current of a recently reported CNT transistor SPICE model from Stanford University [17], [18]. DC sweep simulations were carried out with the gate voltage of 0V to 0.6V with 0.1V step and drain-source voltage 0V to 0.6V with 0.01V step. Both models implement near-ballistic transport. Discrepancies in the \( I_{DS} \) current values can be explained by the fact that the Stanford model considers subband effects which reduce the current [17], [18].

The spline model has the potential to include arbitrary non-ballistic effects in and therefore can be used to predict the performance of non-ideal CNT transistors. Figure 4 shows the \( I_{DS} \) characteristics of the n-type-like CNT transistor implemented in HSPICE with the elastic scattering effect [18] and the strain effect on the channel region [19]. Neither of these effects is included in the Stanford model. The strain effect can change the band gap of the CNT channel and thus reduce the drain current, which matches the output results of the model. It can be seen from the graphs in Figure 4 that the proposed HSPICE model matches more closely the experimental results presented in Figure 5, especially in terms of the saturation region region slope, than the Stanford model.

Additionally, to verify the accuracy of the proposed macromodel, recently reported experimental characteristics [20] were compared with the spline-based model for \( d = 1.6\, \text{nm}, t_{ox} = 50\, \text{nm}, T = 300\, \text{K} \) and \( E_F = -0.05\, \text{eV} \) and presented in Figure 5. It also shows the performance of the Stanford model under the same conditions. The results show a close match between the proposed cubic spline macromodel and experimental measurements, which is more accurate than the Stanford model while maintaining similar speed as shown in Table I.

A corresponding p-type-like CNT transistor has also been implemented in HSPICE and Figure 6 illustrates the corresponding \( I_{DS} \) characteristics. Both n-type-like and p-type-like models were used in an analysis of a complementary CMOS-like CNT inverter. The bulk voltage has also considered to take into account the effects on the charge densities generated by the substrate voltage, which is important to reflect correctly the behaviour of p-type-like CNT transistor.

The HSPICE simulation results of the complementary inverter are shown in figure 7. The figure shows the transfer characteristic calculated by using a ramp voltage as the input signal.

The HSPICE macromodel code for the parameter library and transistor macromodel is shown below.
TABLE I
AVERAGE RMS ERRORS AND CPU TIME IN $I_{DS}$ COMPARISON TO THE EXPERIMENTAL RESULTS OF FETTOY MODEL AND THE PROPOSED NON-BALLISTIC (NB) MODELS FOR $d = 1.6\text{nm}$, $t_{ox} = 50\text{nm}$, $T = 300\text{K}$ AND $E_F = -0.05\text{eV}$.

<table>
<thead>
<tr>
<th>$V_G$[V]</th>
<th>Proposed Macromodel $n = 4$</th>
<th>Stanford Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>13.3%</td>
<td>35.7%</td>
</tr>
<tr>
<td>0.4</td>
<td>12.5%</td>
<td>29.6%</td>
</tr>
<tr>
<td>0.6</td>
<td>11.3%</td>
<td>25.2%</td>
</tr>
<tr>
<td>CPU Time[s]</td>
<td>40.32</td>
<td>47.60</td>
</tr>
</tbody>
</table>

Fig. 6. Drain current characteristics for a p-type CNT transistor HSPICE macromodel.

Fig. 7. Inverter simulation result in HSPICE; input ramps from 0V to 0.6V.

* CNT transistor model using 4-piece cubic spline
* File name: cntmodel.sp

$\text{***** Global parameters *****}$

$\text{***** Library name: param.lib *****}$

$\text{***** Beginning of circuit and device definitions *****}$

$\text{***** Supplies and voltage params: *****}$

$\text{***** Some CNFET parameters: *****}$

$\text{***** Main Circuits *****}$

$\text{***** Measurements *****}$
The complete code for the proposed HSPICE model is now available on the Southampton Carbon Nanotube Transistor Modelling website [21] and available for public use.

IV. CONCLUSION

This paper proposes an HSPICE implementation of the cubic spline based numerically efficient CNT transistor model. HSPICE simulation results match closely those from MATLAB simulations and also recently published experimental measurements. Results show that the accuracy of the proposed HSPICE implementation is superior to that of the state-of-the-art CNT SPICE model developed at Stanford University, while maintaining similar simulation speed. The accuracy of the proposed model can be further increased by inclusion of other physical effects, specifically non-ballistic transport. To demonstrate the feasibility of adding non-ballistic effects, a version of the model has been developed and implemented in HSPICE to include elastic scattering and the strain effect.

V. ACKNOWLEDGEMENT

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