A novel numerical approach to heterojunction bipolar transistors circuit simulation

Yiming Li a,b,*, Kuen-Yu Huang c

a National Nano Device Laboratories, Hsinchu 300, Taiwan
b Microelectronics and Information Systems Research Center, National Chiao Tung University, Hsinchu 300, Taiwan
c Institute of Electronics, National Chiao Tung University, Hsinchu 300, Taiwan

Received 9 August 2002; accepted 25 November 2002

Abstract

In this paper we present a novel computational method for calculating the heterojunction bipolar transistor (HBT) physical characteristics in the time domain. To calculate the HBT high frequency properties, the Gummel–Poon equivalent circuit model is applied to replace the HBT in the circuit and a set of governing ordinary differential equations (ODEs) is formulated. We directly decouple the system ODEs and solve each decoupled ODE with the monotone iterative method in the time domain. This solution methodology proposed here has been applied to semiconductor device simulation by us earlier, and we find this method for the HBT simulation has good accuracy and converges globally. Compared with the HSPICE circuit simulator results, our results present the accuracy, efficiency, and robustness of the method.

© 2002 Elsevier Science B.V. All rights reserved.

PACS: 73.40.Kp; 72.30.+q; 07.05.Tp; 02.60.Cb; 02.30.Hq
Keywords: HBT; ODE; Computer simulation; Monotone iterative method

1. Introduction

Due to the extremely high linearity of HBTs operating at high frequency, these semiconductor devices and structures have been of great interest for physical applications, such as wireless communications in recent years [1–4]. The harmonic balanced method [5–8] is a way for the solution of the HBT ODEs in the frequency domain. This frequency domain approach has some merits, but it has also limitations in studying the physical properties of HBTs with time evolution. Contrary to those solution methods in the frequency domain, another computational alternative to analyze the physical behavior for an HBT device is to solve a set of equivalent circuit ODEs in the time domain directly. Together with the fast Fourier transformation (FFT), the time domain approach can be extended to study the HBT high frequency properties in the time and frequency domain at the same time. The discretized ODEs in circuit simulation are solved traditionally with the Newton’s iterative (NI) method [9]. It is
well known that the NI method is a local method; in general, it converges quadratically in a sufficiently small neighborhood of the exact solution. For example, the famous HSPICE circuit simulator \[10,11\] applied the NI method in the solution of nonlinear system.

In this paper, a novel simulation method for HBT physical characteristics calculations in the large-scale time domain is proposed. This approach mainly uses the monotone iterative (MI) method \[12–19\] instead of the NI method to solve the ODEs. The MI method has been successfully developed and applied to semiconductor device simulation by us earlier \[12–17\]. Based on the decoupling procedure (so-called the waveform relaxation (WR) method \[20\]) and MI method, the HBT circuit ODEs are directly solved in the time domain. The computed time domain results are then analyzed with the FFT to obtain the necessary information in frequency domain. This approach is strongly dependent on the robustness of the nonlinear ODE solver; compared with the conventional NI method, this method converges globally and is inherently parallel. First of all, a set of ODEs are decoupled with the decoupling algorithm. Each decoupled nonlinear ODE is then solved directly with the MI technique and the Runge–Kutta (RK) method. The proposed computational approach has been successfully implemented on a PC-based cluster with message passing interface (MPI) library \[21\]. The primary parallel results show that a well-designed parallel algorithm can reduce the execution time up to an order of magnitude.

This paper is organized as follows. Section 2 states the HBT ODE model, and introduces computational procedure. Section 3 presents the simulation results. Section 4 draws the conclusions.

2. An HBT circuit model and simulation method

As shown in Fig. 1(a), based on the node current flow conservation (the well-known Kirchhoff’s current law) and utilize the Gummel–Poon large signal equivalent circuit model (Fig. 1(b)) for the HBT device \[9,22,23\], the complete simulation model can be formulated with nodal equations. The system of node equations for time dependent HBT circuit is a set of nonlinear coupled ODEs. At nodes C, E, and B we have the following differential equations (1)–(3), respectively.

\[
C_{JCX} \left( \frac{dV_{BX}}{dt} - \frac{dV_C}{dt} \right) + C_{DR} \left( \frac{dV_B}{dt} - \frac{dV_C}{dt} \right) + C_{JCI} \left( \frac{dV_B}{dt} - \frac{dV_C}{dt} \right) \\
+ I_2 + I_{BL2} - \frac{I_{CT}}{q_1 + \sqrt{(\frac{q_1}{2})^2 + q_2}} + \frac{V_{CX} - V_C}{R_C} = 0,
\]

\[
C_{DF} \left( \frac{dV_B}{dt} - \frac{dV_E}{dt} \right) + C_{JE} \left( \frac{dV_B}{dt} - \frac{dV_E}{dt} \right) + I_1 + I_{BL1} \\
+ \frac{I_{CT}}{q_1 + \sqrt{(\frac{q_1}{2})^2 + q_2}} + \frac{V_{EX} - V_E}{R_C} = 0,
\]

\[
C_{DR} \left( \frac{dV_B}{dt} - \frac{dV_C}{dt} \right) + C_{JCI} \left( \frac{dV_B}{dt} - \frac{dV_C}{dt} \right) + C_{DF} \left( \frac{dV_B}{dt} - \frac{dV_E}{dt} \right) \\
+ C_{JE} \left( \frac{dV_B}{dt} - \frac{dV_E}{dt} \right) + I_1 + I_{BL1} + I_2 + I_{BL2} + \frac{V_B - V_{BX}}{RB} = 0.
\]

Similarly, at nodes BX, CX, and EX we formulate, respectively, the equations as follows:

\[
C_{JCX} \left( \frac{dV_C}{dt} - \frac{dV_{BX}}{dt} \right) + \frac{V_B - V_{BX}}{R_B} + \frac{(V_{IN} + V_{in}) - V_{BX}}{R_{B2}} = 0,
\]
Fig. 1. (a) The HBT circuit for the high frequency simulation, (b) a plot of the Gummel–Poon equivalent circuit model for the HBT device.

\[ \frac{V_C - V_{CX}}{R_C} + \frac{V_{CC} - V_{CX}}{R_{CCS}} = 0, \]
\[ \frac{V_E - V_{EX}}{R_E} - \frac{V_{EX}}{R_{EE}} = 0. \]

Eqs. (1)–(4) are the ODEs, and Eqs. (5) and (6) are the algebraic equations. These equations are subject to proper initial values at time \( t = 0 \) for all unknowns to be solved. All currents \( I \) and capacitances \( C \) above are nonlinear functions of unknown variables. These nonlinear terms are

\[ I_1 = \frac{I_S}{B_F} \left[ \exp \left( \frac{V_B - V_E}{N_F V_T} \right) - 1 \right], \]
\[ I_2 = \frac{I_S}{B_R} \left[ \exp \left( \frac{V_B - V_C}{N_R V_T} \right) - 1 \right], \]
\[ I_{BL1} = I_{SE} \left[ \exp \left( \frac{V_B - V_E}{N_E V_T} \right) - 1 \right], \]
\[ I_{BL2} = I_{SC} \left[ \exp \left( \frac{V_B - V_C}{N_C V_T} \right) - 1 \right], \]
\[ I_{CT} = -I_S \left[ \exp \left( \frac{V_B - V_C}{N_R V_T} \right) - \exp \left( \frac{V_B - V_E}{N_F V_T} \right) \right], \]
\[ C_{DR} = \frac{\partial}{\partial(V_B - V_C)} \left[ T_R I_S \exp \left( \frac{V_B - V_C}{N_R V_T} \right) \right]. \]
\[ C_{DF} = \frac{\partial}{\partial(V_B - V_E)} \left\{ \frac{\tau_F I_S [\exp\left(\frac{V_B - V_E}{M_F V_T}\right) - 1]}{\frac{q_1}{2} + \sqrt{\left(\frac{q_1}{2}\right)^2 + q_2}} \right\}, \]  

(13) 

\[ C_{JE} = \begin{cases} 
C_{JEO} \left( 1 - \frac{V_B - V_E}{V_{JE}} \right)^{-M_{JE}}, & \text{if } (V_B - V_E) \leq F_C V_{JE}, \\
C_{JEO} (1 - F_C)^{-M_{JC}} \left[ 1 - F_C (1 + M_{JC}) + \frac{M_{JE}}{V_{JE}} (V_B - V_E) \right], & \text{if } (V_B - V_E) > F_C V_{JE}, 
\end{cases} \]  

(14) 

\[ C_{JCX} = \begin{cases} 
(1 - X_{JCX}) C_{JCO} \left( 1 - \frac{V_{BX} - V_C}{V_{JC}} \right)^{-M_{JC}}, & \text{if } (V_{BX} - V_C) \leq F_C V_{JC}, \\
(1 - X_{JCX}) C_{JCO} (1 - F_C)^{-M_{JC}} \left[ 1 - F_C (1 + M_{JC}) + \frac{M_{JC}}{V_{JC}} (V_{BX} - V_C) \right], & \text{if } (V_{BX} - V_C) > F_C V_{JC}, 
\end{cases} \]  

(15) 

\[ C_{JCI} = \begin{cases} 
X_{JCX} C_{JCO} \left( 1 - \frac{V_B - V_C}{V_{JC}} \right)^{-M_{JC}}, & \text{if } (V_B - V_C) \leq F_C V_{JC}, \\
X_{JCX} C_{JCO} (1 - F_C)^{-M_{JC}} \left[ 1 - F_C (1 + M_{JC}) + \frac{M_{JC}}{V_{JC}} (V_B - V_C) \right], & \text{if } (V_B - V_C) > F_C V_{JC}, 
\end{cases} \]  

(16) 

where \( V_T = \frac{kT}{q} \) is thermal voltage; \( q_1, q_2 \) and \( \tau_F \) are as follows:

\[ q_1 = 1 + \frac{V_B - V_E}{V_{AR}} + \frac{V_B - V_C}{V_{AF}}. \]  

(17) 

\[ q_2 = \frac{I_S}{I_{RF}} \left[ \exp\left(\frac{V_B - V_E}{N_F V_T}\right) - 1 \right] + \frac{I_S}{I_{RR}} \left[ \exp\left(\frac{V_B - V_C}{N_R V_T}\right) - 1 \right], \]  

(18) 

\[ \tau_F = T_F \left[ 1 + X_{TF} \left( \frac{I_{HF}}{I_{HF} + I_{TF}} \right)^2 \exp\left(\frac{V_B - V_C}{1.44 V_{TF}}\right) \right]. \]  

(19) 

The model parameters above for the In_{0.49}Ga_{0.51}P/GaAs HBT in our simulation are listed in Table 1. There are 4 coupled ODEs with the nonlinear current and capacitance models have to be solved and the unknowns to be calculated in the system of ODEs are \( V_C, V_E, V_B, V_{BX}, V_{CX}, \) and \( V_{EX} \), respectively. We note that the system consists of strongly coupled nonlinear ODEs, due to the exponential dependence of current and capacitance models [1,20,22].

We propose here a decoupled and globally convergent simulation technique to solve the system ODEs in the large-scale time domain directly. Firstly, under the steady state condition, we find the DC solution as the starting point to compute other time dependent solutions. For a specified time period \( T \), to solve these nonlinear ODEs in the time domain, our approach consists of following steps:

(i) Let an initial time step \( t \) be given.

(ii) Use the decoupling method to decouple all Eqs. (1)–(6).
Table 1
A list of the parameters used in the modeling and simulation

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Numeric value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>BF</td>
<td>86.95</td>
<td>–</td>
</tr>
<tr>
<td>BR</td>
<td>1.47</td>
<td>–</td>
</tr>
<tr>
<td>CJC0</td>
<td>24.27E–15</td>
<td>F</td>
</tr>
<tr>
<td>CJE0</td>
<td>130.06E–15</td>
<td>F</td>
</tr>
<tr>
<td>FC</td>
<td>0.50</td>
<td>–</td>
</tr>
<tr>
<td>IJKF</td>
<td>0.1815</td>
<td>A</td>
</tr>
<tr>
<td>IJKR</td>
<td>1.032E–3</td>
<td>A</td>
</tr>
<tr>
<td>IS</td>
<td>2.85E–24</td>
<td>A</td>
</tr>
<tr>
<td>IJSC</td>
<td>2.142E–14</td>
<td>A</td>
</tr>
<tr>
<td>IJSE</td>
<td>2.34E–18</td>
<td>A</td>
</tr>
<tr>
<td>ITC</td>
<td>419.80E–3</td>
<td>A</td>
</tr>
<tr>
<td>MSJC</td>
<td>0.266</td>
<td>–</td>
</tr>
<tr>
<td>MSJE</td>
<td>0.1188</td>
<td>–</td>
</tr>
<tr>
<td>NC</td>
<td>1.954</td>
<td>–</td>
</tr>
<tr>
<td>NE</td>
<td>1.910</td>
<td>–</td>
</tr>
<tr>
<td>NF</td>
<td>1.068</td>
<td>–</td>
</tr>
<tr>
<td>NR</td>
<td>1.060</td>
<td>–</td>
</tr>
<tr>
<td>Rb</td>
<td>48.130</td>
<td>Ohm</td>
</tr>
<tr>
<td>RBE2</td>
<td>8.750</td>
<td>Ohm</td>
</tr>
<tr>
<td>RC</td>
<td>6.750</td>
<td>Ohm</td>
</tr>
<tr>
<td>Rg</td>
<td>1.256</td>
<td>Ohm</td>
</tr>
<tr>
<td>TF</td>
<td>2.680E–12</td>
<td>second</td>
</tr>
<tr>
<td>TR</td>
<td>350.06E–12</td>
<td>second</td>
</tr>
<tr>
<td>VJC</td>
<td>0.7161</td>
<td>V</td>
</tr>
<tr>
<td>VJE</td>
<td>1.3670</td>
<td>V</td>
</tr>
<tr>
<td>VTF</td>
<td>66.0000</td>
<td>–</td>
</tr>
<tr>
<td>XJC</td>
<td>0.3428</td>
<td>–</td>
</tr>
<tr>
<td>XTF</td>
<td>275.6000</td>
<td>–</td>
</tr>
</tbody>
</table>

(iii) Each decoupled ODE is solved sequentially with the MI and RK methods.

(iv) Convergence test for each MI loop.

(v) Convergence test for overall outer loop.

(vi) If the specified stopping criterion is reached for the outer loop, then go to step (vii), else update the newer results and back to step (iii).

(vii) If $t < T$, $t = t + \Delta t$ and repeat the steps (iii)–(vi) until the time step meets the specified time period $T$.

For a given specified time step $t$ and the previous calculated results (i.e. results at time step $t - 1$), Fig. 2 is the flowchart of the proposed simulation procedure for the solutions $(V_C, V_E, V_B, V_{BX}, V_{CX}, V_{EX})$ in the large-scale time domain simulation. In step (ii), the decoupling algorithm solves the circuit equations sequentially, for instance, the $V_C$ in Eq. (1) is solved for given the previous results $(V_E, V_B, V_{BX}, V_{CX}, V_{EX})$. The $V_E$ in Eq. (2) is solved for newer given $V_C$ and $(V_B, V_{BX}, V_{CX}, V_{EX})$. The $V_B$ in Eq. (3) is solved for newer given $(V_C, V_E)$ and $(V_{BX}, V_{CX}, V_{EX})$. We have similar procedure for other unknowns [13,17,19,20]. We use the DC solutions and previous calculated results as the starting point for all unknowns to be solved at present time step $t$. This method converges globally and is not sensitive to the initial guesses in the solution process [19].

Each decoupled ODE is solved with the MI algorithm. To clarify the MI algorithm for the numerical solution of the decoupled nonlinear ODEs, we write the above ODEs as the following form

$$
\frac{dV_X}{dt} = f(V_X, t),
$$

(20)
Fig. 2. A flowchart of the proposed simulation methodology.
where \( V_X \) is the unknowns to be solved and \( f \) is the collection of the nonlinear functions. We define the MI parameter \( \lambda = \frac{\partial f}{\partial V_X} \) [13,17–19] and inserted the \( \lambda \) into Eq. (20), then we have the MI equation
\[
\frac{dV_X}{dt} = f(\eta, t) - \lambda(V_X - \eta), \tag{21}
\]

where \( v_0 \leq \eta \leq w_0 \) is a value in \([0, T]\), and \( v_0 \) and \( w_0 \) are the lower and upper solutions of Eq. (20), respectively [18,19]. Based on the nonlinear behaviors of each decoupled circuit ODEs, mathematically we have shown that the solution algorithm has monotone convergence property [19]. As shown in Fig. 2, we solve Eq. (21) with respect to each unknown using the RK method, where the notation subscript \( o \) is the previous iteration results, and the superscripts \((t - 1)\) and \((t)\) represent the previous and present time steps. The nonlinear functions \( F_i(\cdot), i = 1, \ldots, 6 \) are the corresponding nonlinear terms of the ODEs above, where the TOL is the error tolerance, \( h \) is the increment in the RK formula of fourth order [24].

Fig. 3 shows the achieved convergence properties (maximum norm error versus number of outer iterations) on the proposed method for the HBT simulation, where the \( V_{\text{IN}} = 1.42 \) V and \( V_{\text{CC}} = 5 \) V. In our calculation experience, a convergence criterion for all quantities (maximum norm error \( < 10^{-10} \) and \( 10^{-7} \) for the inner and the overall outer loops) can be reached by only 8–12 MI loops and 25–30 outer loops, respectively. The simulation time is an important consideration in circuit simulation. Under the same convergence criterion above, a comparison of the simulation CPU time between our developed simulator and HSPICE simulator is performed on a PC-based Linux workstation (CPU is with Pentium-IV 1 GHz and RAM = 512 MBytes). In the comparison, 40 cycles are computed, the input amplitude of two-tone signal \( V_m = 0.002 \) V, and the frequencies \( f_1 \) and \( f_2 \) are 1.71 and 1.89 GHz, respectively. As shown in Table 2, we find the simulation time of two simulations is in the same order magnitude. For a fixed convergence criterion, simulation time of our method increases linearly when the number of simulation points per cycle are increased. Furthermore, our method can be easily implemented on a Linux-cluster
for a parallel speedup. Based on the global convergence of the MI method, we can solve all jobs independently, and hence this algorithm is inherently parallel in the time domain analysis. For an HBT circuit simulation at 1.0 GHz with 40 waveform periods, the achieved parallel speedup factor is about 6.4 on an 8-PCs based Linux-cluster with MPI library [15].

3. Results and discussion

The DC characteristics of the HBT circuit shown in Fig. 1 is performed firstly, and the computed results are inputted as starting points in high frequency simulation. In our simulations, computed family DC curves with our method demonstrate very good consistence with the results from the well-known HSPICE simulation.

For the nonlinearity analysis of the equivalent HBT circuit, we calculate the two-tone input signal in the time domain with intermodulation. The simulation was done directly in the time domain relies on the robustness of the developed circuit simulator with the MI method. From the computed periodic output results, we found the output signal has good repetition. Fig. 4 shows the calculated output voltage ($V_{OUT}$) in the time domain with a
two-tone input signal. As shown in Fig. 1, the input signal $V_{IN}$ is the DC bias and the expression of $V_{in}$ is as follows: $V_{in} = V_m \sin(2\pi f_1 t) + V_m \sin(2\pi f_2 t)$, where the $V_m = 0.002$ V, and the frequencies $f_1$ and $f_2$ are 1.71 and 1.89 GHz, respectively. Figs. 4 and 5 are our results and the HSPICE results, respectively. Contrary to the HSPICE results initially have some unstable calculations, our simulator presents its robustness in the large signal time domain analysis. We convert the time domain results into the frequency with the FFT directly. Figs. 6 and 7 are the corresponding results with Figs. 4 and 5, respectively. We find the products of the third-order intermodulation (IM3) at $2f_1 - f_2$ and $2f_2 - f_1$ are clearly observed in Fig. 6. However, as shown in Fig. 7 it is difficult to identified the two IM3 products. Our methodology for large scale time domain analysis and two-tone intermodulation demonstrates its superiority over some approaches. Compared to conventional NI-based circuit simulation methodology (e.g.,

![Fig. 6. The output power versus frequency. The results are calculated with our time domain results and FFT.](image1)

![Fig. 7. The frequency domain results from the HSPICE simulation. The IM3 products cannot be identified from this calculation.](image2)
HSPICE), our approach provides a novel alternative in studying the physical properties of transistors and is useful for modern microelectronic system simulation.

4. Conclusions

A novel circuit simulation based on the waveform relaxation and monotone iterative methods has been proposed. With this approach, the DC and two-tone AC characteristics for an HBT circuit were directly computed from time domain results. Compared with the HSPICE simulator, our solution method for an HBT high frequency simulation has been presented to show the accuracy and efficiency of the method. This method provides an alternative for the time domain solution of circuit ODEs. This solution methodology can be generalized for larger circuit simulation including more transistors.

Acknowledgements

This work was supported in part by the National Science Council of Taiwan, under contract number NSC 91-2112-M-317-001 and the 2002 Research Fellowship Award of the Pan Wen-Yuan Foundation in Taiwan.

References