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Algorithms for "Curve-Tracer" Mode in Simulation of Devices with Highly Nonlinear Characteristics

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EXTENDED ABSTRACT

Introduction

Traditional device simulators compute the device characteristics, including I-V curves and device parameters, based on the user-specified bias points. The computation efficiency is low with such an approach when a whole family of curves are to be generated because the linearity of the device behavior in certain operation regions has not been explored. On the other hand, it is not uncommon that simulators perform poorly in terms of convergence rate and robustness in Newton iterations when devices operate in highly-nonlinear regions. These two drawbacks can be overcome by evaluating also the first-order derivatives of I-V characteristics during the solution process. In fact, the Jacobian matrix from the Newton iteration can be viewed as the linear model to the nonlinear system under simulation at the current operation point. The exploration of this linear model to the maximum extent can not only help determining the biases needed to resolve the device characteristics, but also can improve the convergence behavior of device simulators.

In this paper, three numerical techniques are introduced to achieve above goals. They are the relaxed Newton projection method (NPM) [1], the determination of closeness of the initial guess to the final solution or, say, the degree of linearity of device behavior in certain operation region, and the dynamic formulation of Jacobian matrix. The implementation of these techniques in PISCES [2] and SEDAN [3] has led to efficient simulation of two types of highly-nonlinear devices -- GaAs MESFETs employing negative-differential-mobility model [4], and $Si/Si_{1-x}Ge_x$ HBTs.

Definition of Two Numerical Criteria

We define in this section two quantitative criteria useful for the numerical simulation of device characteristics. First, the resolution of I-V curves, i.e. the fineness to which a curves can reveal the essential feature of the device. For example, for a linear segment of the device I-V curve, two bias points would be enough to characterize the entire feature, whereas in a nonlinear region, more biases are needed to achieve the same degree of resolution. This fact suggests that the change of slopes rather than that of values of dependent variables should be used as the measure of resolution. The resolution of a curve, α, is defined as

$$\ln(\alpha) = \left| \ln \frac{s_{i+1}}{s_i} \right| = \left| \ln(s_{i+1}) - \ln(s_i) \right| \tag{1}$$

where i and $i+1$ represent adjacent bias points, and the value of s is always taken as the positive number.

The second criterion is about the measure of the linearity within an operation region. Since the projection of the initial guess from the previous solution using NPM is based on the linear model (Jacobian) at the previous bias, if the device behaves linearly with respect to the bias change within this interval, the initial guess should fall right in the Newton convergence (quadratic rate)

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region. A good measure of the closeness of a trial solution to the real one is the size of update in potential during Newton iterations. Specifically, we suggest to use the potential update less than one tenth of the thermal voltage as a criterion for closeness. After the first iteration at the present bias, if the potential update using initial guess from NPM is smaller than the criterion, one may consider the device behaves linearly within this bias range.

Algorithms

The numerical techniques mentioned above are realized through the following two algorithms. The first one is on the determination of bias points (auto-biasing). It is found that the slope change of a curve is very localized, and the trend of the slope change can be extrapolated based on only two most recent biases. In view of this observation, the auto-biasing algorithm can be formulated as follows. The parameters input from users are resolution α, and the lower and upper limits for bias steps, l and u.

1. Starting from the first bias point (usually zero bias), find the exact solution using the Newton iteration.
2. Advance an initial bias step of size l.
3. Solution at the new bias point:
   - Get initial guess from solution at the previous bias using NPM.
   - Perform Newton iteration once. If the closeness criterion as stated in the previous section is met, stop iteration. Otherwise continue iterations until the solution is found.
   - check if $\Delta\ln(s) < \ln(\alpha)$. If yes, do next step, otherwise go to step 6.
4. Use the linear extrapolation to compute the next bias step,

$$\Delta V_+ = \frac{\ln(\alpha)}{|\ln(s_{i+1}) - \ln(s_i)|}\Delta V_i \qquad (2)$$

   where ΔV_+ is the new bias step, and $\Delta V_i = V_{i+1} - V_i$ where $i+1$ and i represents the present and previous biases.
5. If $\Delta V_+ > u$ then $\Delta V_+ = u$. If $\Delta V_+ < l$ then $\Delta V_+ = l$. Go back to step 3.
6. The step size is too large, insert a new bias point between the current bias and the previous one. The fraction for the bias step partition can also be specified by the user. Go to step 3.

The above loop is terminated when the final bias given by the user is reached.

The second algorithm is for the improvement of the robustness of the Newton iteration by forming the Jacobian matrix in a gradual fashion. We use the field-dependent mobility as an example to describe this algorithm. The central idea is to "turn on" the field-dependency of mobility in evaluating Jacobians only when the trial solution is close enough to the actual one.

For a new bias, if the closeness criterion is met for the initial guess, continue iterations with the full Jacobian until the convergence is reached. If the first potential update is between 0.1 and 1 V_T, the field-independent Jacobian is first used until the update in potential is either reduced to below 0.01 V_T or decreasing in three consecutive iterations to below 0.2 V_T. Afterwards, the full Jacobian is used until the convergence is reached. If the first update in potential is bigger than V_T, it suggests that the projected initial guess is not good enough. In a highly nonlinear operating region, it is preferable to reduce the bias step in order to avoid unnecessary (and unsuccessful) iterations.

Examples

The following two examples are used as the test cases to above algorithms which have been implemented in both PISCES and SEDAN.

The first one is the simulation of drain current (I_{ds}) vs. drain voltage (V_{ds}) with gate-source bias (V_{gs}) as parameter for GaAs MESFETs using PISCES. The mobility model [4] used has an intrinsic negative differential mobility (NDM) region in the velocity-field curve. The physical structure of the MESFET has the channel doping of $1.2\times10^{17}cm^{-3}$ and the channel length of 2.6μ. Without using the proposed algorithm, the simulator fails to converge for $V_{ds} > 1.85V$, and with bias step size as small as 0.05V, in order to advance V_{ds} by 0.1 volt it still takes several hundred iterations (Table 1). Using the new scheme which combines the auto-biasing and gradual formation of the Jacobian matrix, however, both the computation efficiency and the robustness of the Newton iteration are significantly improved. The comparison of the performance with and without the new algorithms is shown in Table 1. For drain voltage less than 1.8V, the average speed improvement is nine times with maximum of twenty-four times. Above $V_{ds} = 1.8V$, the original program does not work at all, whereas the new one takes about fifty iterations for bias step of 0.1V. The automatically-determined biases are shown in Fig. 1. It can be seen that the complete feature of the curve is reproduced by a few bias points. The negative differential resistance region in the output characteristics is caused by the NDM region in the mobility model used.

V_{dd} (V_{gs}=0)	No. of iterations	
	field-indep.	this scheme
0 - 0.7	214	22
- 0.8	69	7
- 0.85	90	48
- 0.9	140	9
- 1.0	121	25
- 1.1	180	25
- 1.2	149	27
- 1.3	190	32
- 1.4	172	35
- 1.5	256	34
- 1.6	307	32
- 1.7	382	29
- 1.8	608	25

Table 1. Comparison of iteration count

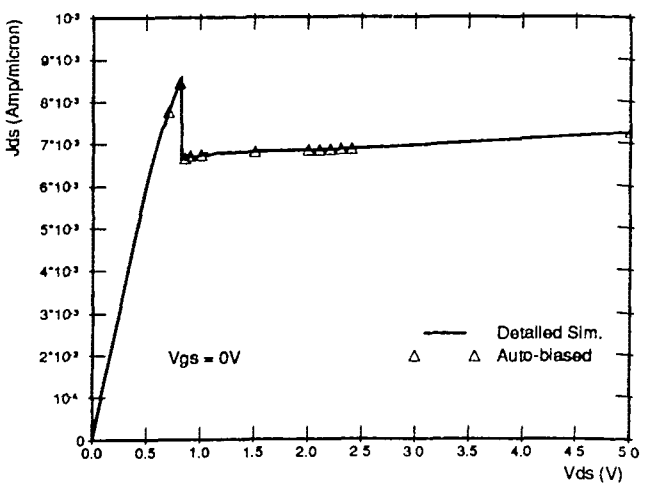

Fig. 1 Simulated output curve of GaAs MESFET

The second example is the simulation of Si/SiGe/Si HBTs with the narrow-bandgap base region using SEDAN. As is discussed in [5], for double heterojunction bipolar transistors, there exists a kink in the collector current at high-level injection, so the J_c vs. V_{be} curve in Gummel plot is highly nonlinear for bigger V_{be}. As is shown in Fig. 2, the proposed auto-biasing scheme catches the device feature very well by placing more bias points where they are needed to resolve the fine feature. Also shown in Fig. 3 is the output curve with V_{be} as parameter. In both examples, α is chosen as 1.5 (with ±0.15 tolerance), and the maximum bias step allowed in Fig. 2 is $u = 0.5V$, whereas in obtaining Fig. 3 l is set to 0.1V.

Conclusions

The proposed algorithms enable device simulators be turned into "curve-tracers", which are highly desirable for both device design and circuit simulation. Moreover, the enhanced convergence behavior of the NR method has many potential applications in other hard-to-converge problems employing such physical mechanisms as the carrier impact ionization and carrier-concentration dependent bandgap narrowing.

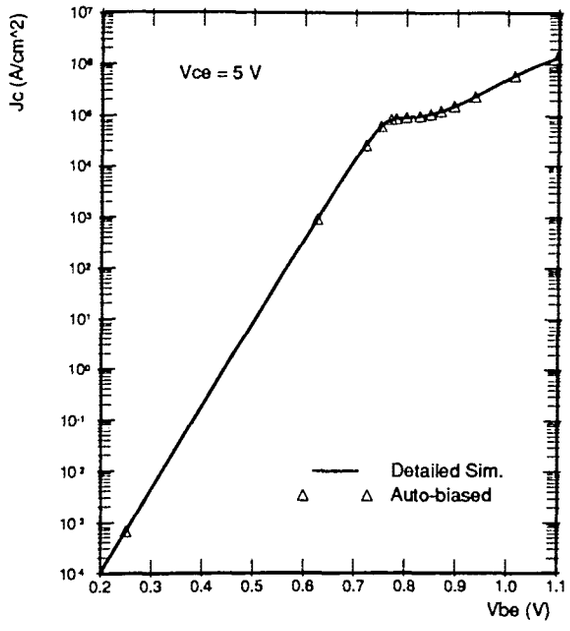

Fig. 2 Simulation of J_c vs. V_{be} for Si/SiGe/Si HBT

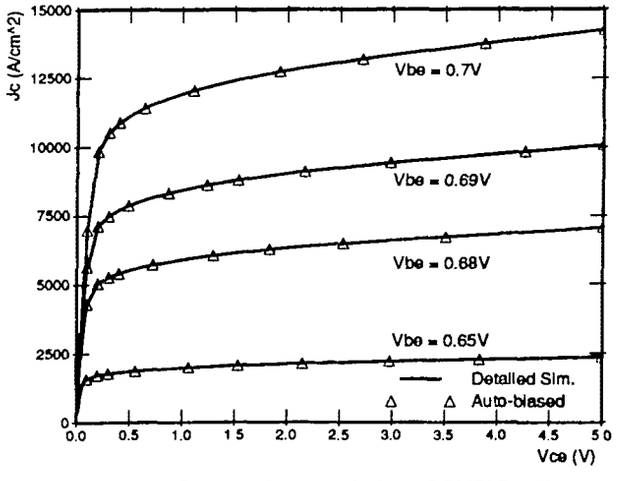

Fig. 3 Output characteristics of Si/SiGe/Si HBT

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