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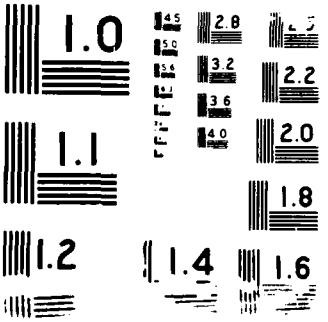
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WAVEFORM RELAXATION APPLIED TO TRANSIENT DEVICE SIMULATION

M. Reichelt, J. White, J. Allen, and F. Odeh

Abstract

In this paper we investigate the possibility of accelerating the transient simulation of MOS devices by using waveform relaxation. Standard spatial discretization techniques are used to generate a large, sparsely-connected system of algebraic and ordinary differential equations in time. The waveform relaxation (WR) algorithm for solving such a system is described, and several theoretical results that characterize the convergence of WR for device simulation are given. In addition, one-dimensional experimental results are presented.

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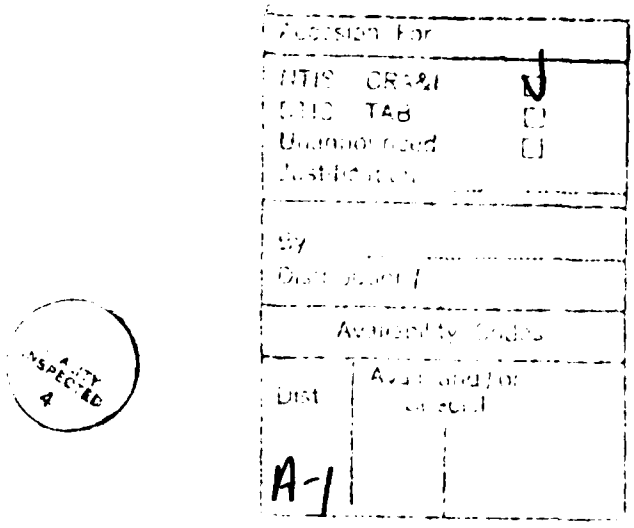

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Waveform Relaxation Applied to Transient Device Simulation

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Abstract

In this paper we investigate the possibility of accelerating the transient simulation of MOS devices by using waveform relaxation. Standard spatial discretization techniques are used to generate a large, sparsely-connected system of algebraic and ordinary differential equations in time. The waveform relaxation (WR) algorithm for solving such a system is described, and several theoretical results that characterize the convergence of WR for device simulation are given. In addition, one-dimensional experimental results are presented.

1 Introduction

Both digital and analog MOS circuit designers rely heavily on circuit simulation programs like SPICE [3] to insure the correctness and to test the performance of their designs. For most applications, the lumped MOS models used in these programs [9] accurately reflect the behavior of terminal currents and charges, but in some cases, these models are not adequate. In particular, charge redistribution between source and drain during device switching cannot easily be modeled by a lumped device, but the details of this charge redistribution can have an important effect on circuit behavior. In circuits like dynamic memory cells, sense amplifiers, analog-to-digital converters, and high frequency operational amplifiers, charge redistribution effects may not only degrade performance, but can inhibit proper function.

For these critical applications, sufficiently accurate transient simulations can be performed if, instead of using a lumped model for each transistor, the transis-

tor terminal currents and charges are computed by numerically solving the drift-diffusion based partial differential equation approximation for electron transport in the device. However, simulating even a few transistor circuit in this way is very computationally expensive, because the accurate solution of the transport transport equations an MOS device requires a two dimensional mesh with more than a thousand points.

In this paper we investigate the possibility of accelerating the transient simulation of MOS devices by using waveform relaxation. In the next section we start by introducing the equations for transient device simulation. Then we view the result of applying commonly used spatial discretization techniques to these equations, generating a large, sparsely-connected system consisting of algebraic and ordinary differential equations in time. In Section 3 we present the waveform relaxation algorithm for solving such a system, and suggest why it may be particularly efficient. Several theoretical results that characterize the convergence of the method are presented in Section 4, and one-dimensional experimental results are described in section 5. Finally, conclusions and acknowledgements are given in section 6.

2 Classical Simulation Equations

The terminal behavior of an MOS device is well described by the Poisson equation and the electron current-continuity equation [5]

$$\epsilon \nabla^2 \psi + q\,(N - n) = 0 \tag{1}$$

$$\nabla \cdot \vec{J}_n - q\frac{\partial n}{\partial t} = 0 \tag{2}$$

In these equations ψ is the electrostatic potential, q is the magnitude of electronic charge, n is the electron concentration, and $\vec{J}_n$ is the electron current density. N is the net doping concentration given by $N = N_D - N_A$ where N_D and N_A are the donor and acceptor concentrations.

The electron current density is commonly approximated by the drift-diffusion equation:

$$\vec{J}_n = -q\,(\mu_n\, n\, \nabla\psi - D_n \nabla n) \tag{3}$$

where μ_n is the electron mobility, and D_n is the diffusion coefficient. An equation system with only n and ψ as unknowns is derived by using (3) to eliminate $\vec{J}_n$ from (2).

There are a variety of ways to spatially discretize the system of two equations in the two unknowns n and ψ. Given a rectangular two dimensional mesh, a common approach is to use a finite-difference formula for the Poisson equation, and an exponentially-fit finite-difference formula for the current-continuity equation. For notational simplicity, we will assume that the mesh points are

evenly spaced a distance l apart, so that the discretized Poisson equation at each mesh point i is:

$$\epsilon \sum_j (\psi_j - \psi_i) + ql^2 (N_i - n_i) = 0 \tag{4}$$

where n_i, ψ_i, and N_i are the electron concentration, the potential, and the net doping concentration at mesh point i. The summation is taken over the nodes j surrounding i (four nodes for a mesh node i not on the boundary, i.e. north, south, east, and west).

Under the same assumptions, and assuming constant mobility, the discretized current-continuity equation with the drift-diffusion approximation becomes:

$$qD_n \sum_j [B(u_j - u_i)n_j - B(u_i - u_j)n_i] - ql^2 \left(\frac{d}{dt} n_i\right) = 0 \tag{5}$$

where $u_i = q\psi_i/KT$ and $B(x) = x/(\exp x - 1)$ is the Bernoulli function used to exponentially fit the potential variation to the electron concentration variation. In this equation, the Einstein relation $D_n = (KT/q)\mu_n$ has been used to eliminate μ_n.

If there are m mesh points, then the result of applying the spatial discretization to (1),(2), and (3) is a sparse system of m algebraic constraints, represented by (4), and a sparsely connected system of m ordinary differential equations, represented by (5).

3 The Waveform Relaxation Process

The standard approach used to solve these two systems is to discretize the $\frac{d}{dt} n_i(t)$ term in (5) with a low order integration method such as backward-Euler [1]. The result is a sequence of algebraic systems in $2m$ unknowns, each of which can be solved with some variant of Newton's method and/or relaxation. Another approach is to apply relaxation directly to the differential equation system. This leads to a time waveform relaxation process, as given by the following algorithm.

Although only the Gauss-Jacobi algorithm is presented for the sake of notational simplicity, a Gauss-Seidel version could be created by adjusting the iteration indexes.

The WR algorithm reduces the problem of simultaneously solving m differential equations and m algebraic equations to one of iteratively solving $2m$ independent equations. Each of the m differential equations for the $n_i(t)$ waveforms can be solved with a numerical integration method such as backward-Euler. Since they only contribute algebraic constraints, the equations for calculating the $\psi_i(t)$ waveforms need to be solved only at the discrete points in time used to calculate the $n_i(t)$ waveforms.

Algorithm 1 WR Gauss-Jacobi Algorithm for solving the system produced by equations (4) and (5).

The superscript k denotes the iteration count, the subscript i denotes the component index of a vector, and ϵ_ψ and ϵ_n are small positive numbers.

$k \leftarrow 0$
repeat {
  $k \leftarrow k + 1$
  foreach$(i \in \{1, \ldots, n\})$ {
    solve

$$\epsilon \sum (\psi_j^{k-1} - \psi_i^k) + ql^2 (N_i - n_i^{k-1}) = 0$$

$$qD_n \sum \left[B(u_j^{k-1} - u_i^{k-1}) n_j^{k-1} - B(u_i^{k-1} - u_j^{k-1}) n_i^k \right]$$

$$-ql^2 \left(\tfrac{d}{dt} n_i^k \right) = 0$$

    for$(\psi_i^k(t), n_i^k(t);\ t \in [0, T], n_i^k(0) = n_{i0})$
  }
} **until**$(\|\psi^k - \psi^{k-1}\| \leq \epsilon_\psi$ **and** $\|n^k - n^{k-1}\| \leq \epsilon_n)$

The inherent advantage of the WR approach is that the differential equations are solved in a decomposed fashion, and therefore different sets of timesteps can be used at different mesh points to calculate the time evolution of the electron concentration. The method exploits multi-rate behavior. In MOS devices, the rate at which electron concentrations evolve may be very different in the channel compared to the source or the drain. Therefore, WR may prove to be efficient for the device simulation problem, provided it converges, and doesn't take too many iterations. This is the subject of the next section.

4 Theoretical Results

As is usually the case for waveform relaxation algorithms applied to systems of differential equations, Algorithm 1 converges to the solution of the differential-algebraic system for any initial guess that matches the initial conditions. The precise statement is given in the following theorem.

Theorem 1 *Given a finite interval* $[0,T]$, *and any initial guess* $n^0(t)$ *and* $\psi^0(t)$, $t \in [0,T]$, *such that* $n^0(0) = n_0$, *the sequence of waveforms produced by Alg. 1 converges to the exact solution of the system given by equations (4) and (5).*

The proof of the above theorem follows the same steps as the Picard-like proofs of waveform relaxation for ordinary differential equations [10]. First the equations that describe the difference between one iteration and the next are organized into the form

$$\delta\psi^{k+1} = A\delta\psi^k + B\delta n^k(t) \tag{6}$$

and

$$\delta n^{k+1}(t) = \int_0^t \left[f(n^{k+1}(t), n^k(t), \psi^k(t)) - f(n^k(t), n^{k-1}(t), \psi^{k-1}(t)) \right] \tag{7}$$

where $\delta\psi_i^k = \psi_i^k - \psi_i^{k-1}$, $\delta n_i^k = n_i^k - n_i^{k-1}$. The matrices $A, B \in \Re^{m\times m}$ and the function $f : \Re^{m\times m\times m} \rightarrow \Re^m$ are constructed from the iteration equations in Alg. 1. The next step is to show that (6) and (7) represent a contraction. To this end, consider an interval of time short enough to insure equation (7) represents a contraction with respect to n for a fixed ψ. That (6) is a contraction with respect to ψ for a fixed n is well-known [8], as (6) represents relaxation applied to the Poisson equation. One can fit the two contractions together to show that relaxation applied to the coupled system converges.

The above proof outline suggests that the WR algorithm converges in a nonuniform manner. That is, first convergence is achieved over a short time interval, set by what is needed to make (7) a contraction, then over the next short time interval, and then the next, continuing slowly, until the convergence is achieved throughout an entire interval of interest. When applied to general

differential equation systems, like circuits, WR does demonstrate this nonuniformity in the convergence [7], but WR does not usually show nonuniformity when applied to the transient device simulation problem.

In order to analyze why this is the case, we will consider a model problem of just the differential equation associated with the electron concentration, n and assume that the potential ψ is known. The WR iteration update equation for this case is then

$$D_n \sum_j \left[B(u_j - u_i) n_j^k - B(u_i - u_j) n_i^{k+1} \right] - l^2 \left(\frac{d}{dt} n_i^{k+1} \right) = 0 \qquad (8)$$

for each $i \in \{1, \ldots, m\}$. Note that given ψ, (8) is a linear time-varying differential equation in n. For this problem we have the following theorem:

Theorem 2 *If at each time t, $\psi(t)$ is such that the electric field along any vertical or horizontal line is either constant, or monotonically increasing, then (8) is a contraction in a uniform norm on any finite interval $[0, T]$. That is,*

$$max_{[0,T]} ||\delta n^{k+1}(t)|| \leq \gamma max_{[0,T]} ||\delta n^k(t)|| \qquad (9)$$

where $\gamma < 1$.

The proof of Theorem 2 is given in the appendix.

Since allowing the different differential equations to take very different timesteps is WR's main advantage, if this property were limited to insure convergence, the WR algorithm would not be effective. Fortunately, that the WR algorithm is a contraction in a unform norm on any interval implies that the timesteps used to numerically integrate the differential equations are almost unconstrained. Given that the different differential equations use different timesteps, interpolation must be used to communicate results between equations, and if not done carefully this can cause nonconvergence. Linear interpolation is certain not cause problems, and therefore we have the following theorem [7]:

Theorem 3 *Let each of the m independent WR iteration update equations given in (8) be solved numerically with backward-Euler, with m different sets of timesteps. In addition, assume that linear interpolation is used to derive values for the n_i's between time discretization points. Then this multirate discretized WR algorithm for (8) converges, regardless of the timestep selections.*

5 One Dimensional Experiments

Except for Theorem 1, the above theoretical results only apply under certain conditions, and are only an indication that the WR algorithm may be effective. In order to verify that the theoretical results apply in actual simulation, a one-dimensional transient device simulation program was written and applied to a

one-dimensional approximation of an MOS device with a conducting channel. The doping distribution for the one-dimensional device is given in Fig. 1, where the tick marks denote the mesh points. Potential and electron concentration boundary conditions were given at $x = 0.0$ and $x = 3.0\mu$. The boundary values for the electron concentration were computed assuming charge neutrality at the "contacts".

The relaxation process was tested by first solving the static problem with zero volts across the "device", and then making a step change of five volts. Even with this simple example, the variable-by-variable WR algorithm as given in Alg. 1 was ineffective. The iterates did not converge in a uniform manner, and they converged very slowly.

In order to improve convergence, rather than using variable-by-variable decomposition, we partitioned the problem into blocks based on two techniques. First, we associated the electron concentration at node i, $n_i(t)$ with the potential $v_i(t)$ at that node. Then, in order to try to satisfy the assumptions of Theorem 2, we placed together neighboring nodes where we expected rapid changes in the electric field. The resulting partitioning of the nodes are boxed in Fig. 1.

The resulting waveform iterations for the slowest converging variable, the electron concentration for the mesh point where the doping changes abruptly, is plotted in Fig. 2. As the figure indicates, with the partitioning just described, the WR process converges in just a few iterations and the contraction is uniform through time as predicted by Theorem 2. The simulation was rerun with very coarse timesteps to see the effects on convergence, and the WR iterations for the same node is plotted in Fig. 3. As the figure indicates, using coarse timesteps does not effect the overall convergence, although the convergence for small t is slowed.

6 Conclusions and Acknowledgements

In this paper we presented some preliminary results that indicate the WR algorithm may indeed be efficient for device transient simulation. In particular, it was shown that under conditions that can be arranged for in practice, the WR algorithm is a contraction in a uniform norm on any interval $[0, T]$. Also, given these same conditions, the relaxation process will still converge even if very different sets of timesteps are used for the individual iteration equations. Finally, we verified the theoretical results on a one dimensional example.

There are several aspects of WR that need to be addressed if this method it to be efficent for two-dimensional MOS transient device simulation. Most important, a general algorithm for blocking the device must be developed. An efficent approach for determining what discretization points to use for the algebraic constraints must be considered. In addition, the efficiency of WR methods can also be improved by refining the timesteps with iterations, or using a single waveform-Newton iteration to solve the nonlinear WR iteration equations.

The authors would like to thank W. Van Bokhoven for suggesting this research area and John Wyatt for his suggestion on the proof of theorem 2. This work was supported by the Defense Advanced Research Projects Agency contract N00014-87-K-825, and the Air Force Office of Scientific Research grant AFOSR-86-0164.

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A Proof of Theorem 2

The WR iteration equations applied to the model problem (8) can be described as

$$\dot{n}^{k+1}(t) = D(t)n^{k+1}(t) + M(t)n^k(t) \tag{10}$$

where $D(t), M(t) \in \Re^{n\times n}$, and $D(t)$ is negative diagonal matrix. The assumptions about the electric field result in values for the Bernoulli functions such that $D(t)$ and $M(t)$ will satisfy the relation

$$\|d_{ii}(t)\| \geq \epsilon_i + \sum_{j\neq i} \|m_{ij}(t)\|. \tag{11}$$

where $\epsilon_i \geq 0$ and is strictly greater than zero for those $i's$ corresponding to the mesh points next to the boundaries. Note that this implies

$$\|D(t)^{-1}M(t)\| \leq \gamma \tag{12}$$

for $\gamma < 1$, for some norm on $\Re^{n\times n}$ and for all t.

Given the relationship between $D(t)$ and $M(t)$, the WR algorithm applied to a system of the form of (13) will contract in a uniform norm. This has been shown for the case when $D(t)$ and $M(t)$ are independent of t, using Laplace transforms [2]. In the time dependent case, the result can be shown by examining the difference between iteration k and $k+1$ of (13) to get

$$\dot{\delta n}_i^{k+1}(t) = d_i i(t)\delta n_i^{k+1}(t) + \sum_{i\neq j} m_{ij}(t)\delta n_j^k(t) \tag{13}$$

for each mesh point i, where $\delta n_i^k(t) = n_i^k(t) - n_i^{k-1}(t)$. By assumption, $d_{ii}(t) < 0$ and $\delta n_i^k(0) = 0$. Therefore,

$$max_{[0,T]}|\delta n_i^{k+1}(t)| \leq \sum_{i\neq j} max_{[0,T]}|\frac{m_{ij}(t)}{d_{ii}(t)}|max_{[0,T]}|\delta n_j^k(t)|. \tag{14}$$

Equation (14) follows from the fact that for all values of $\delta n^{k+1}(t)$ on the boundary of (or outside) the bounded region $\delta n_i^{k+1}(t)$ points back into the bounded region [6].

Assembling the equation system from (14) results in

$$max_{[0,T]}|\delta n^{k+1}(t)| \leq max_{[0,T]}|D(t)^{-1}M(t)|max_{[0,T]}|\delta n^k(t)|. \tag{15}$$

Then in the norm for which $\|D(t)^{-1}M(t)\| \leq \gamma < 1.0$,

$$max_{[0,T]}\|\delta n^{k+1}(t)\| \leq \gamma max_{[0,T]}\|\delta n^k(t)\|. \tag{16}$$

which proves the theorem.

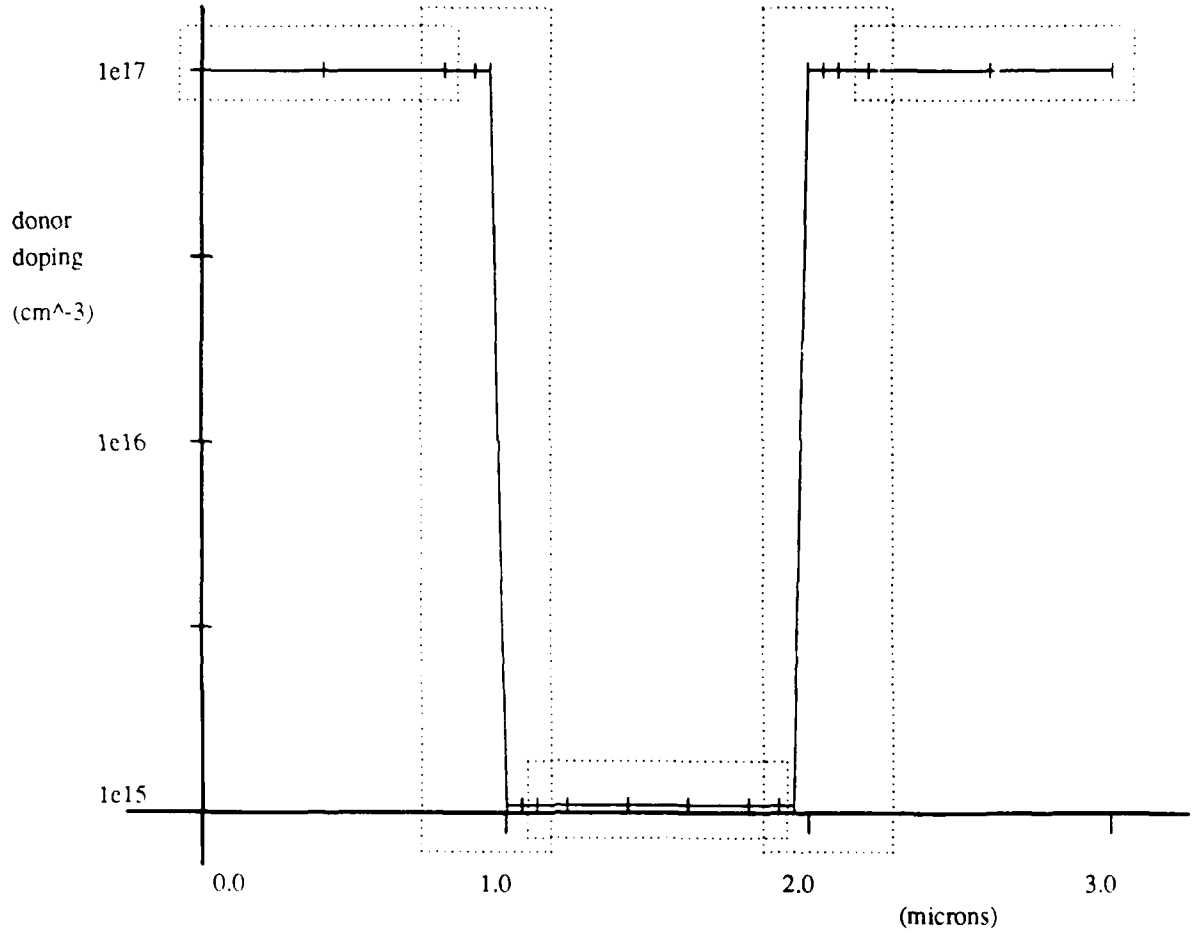

Figure 1: The net doping profile, and the blocking of the mesh points.

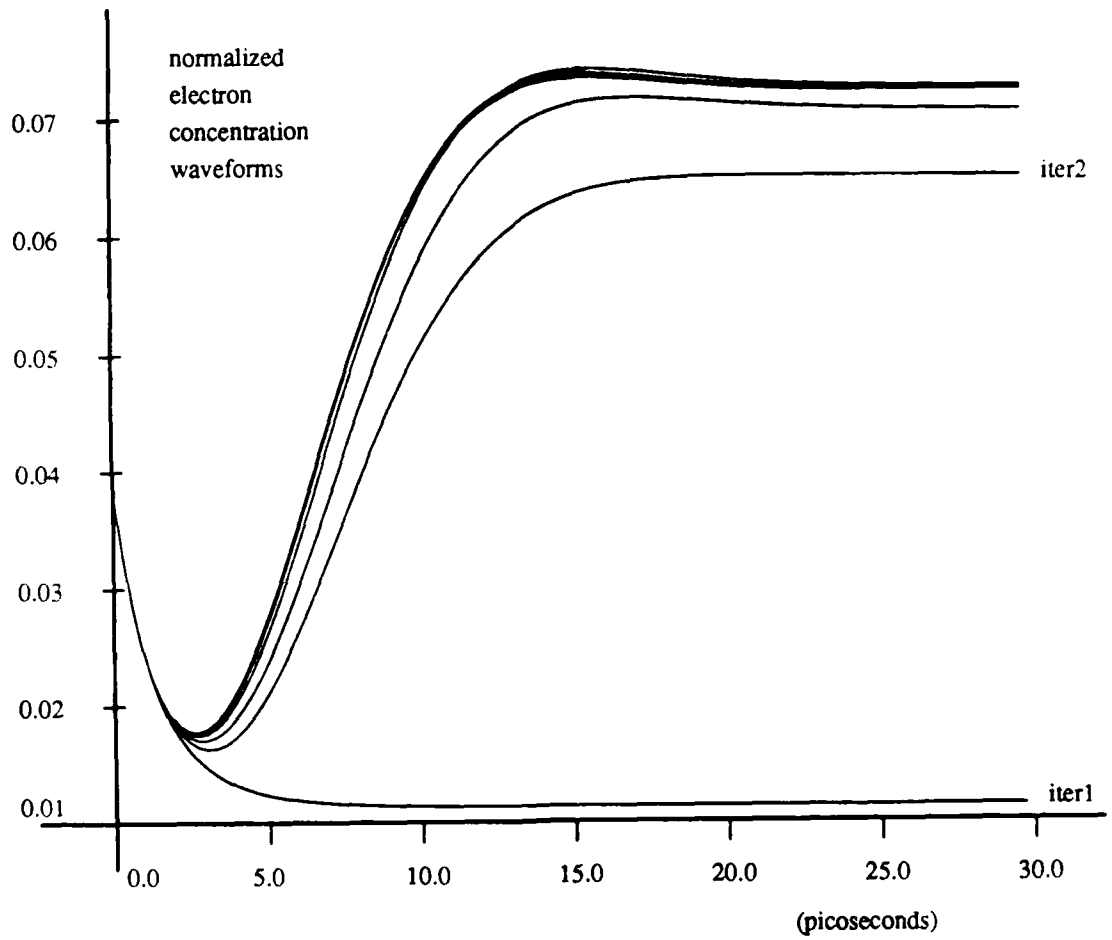

Figure 2: The uniform WR convergence of the electron concentration at a node.

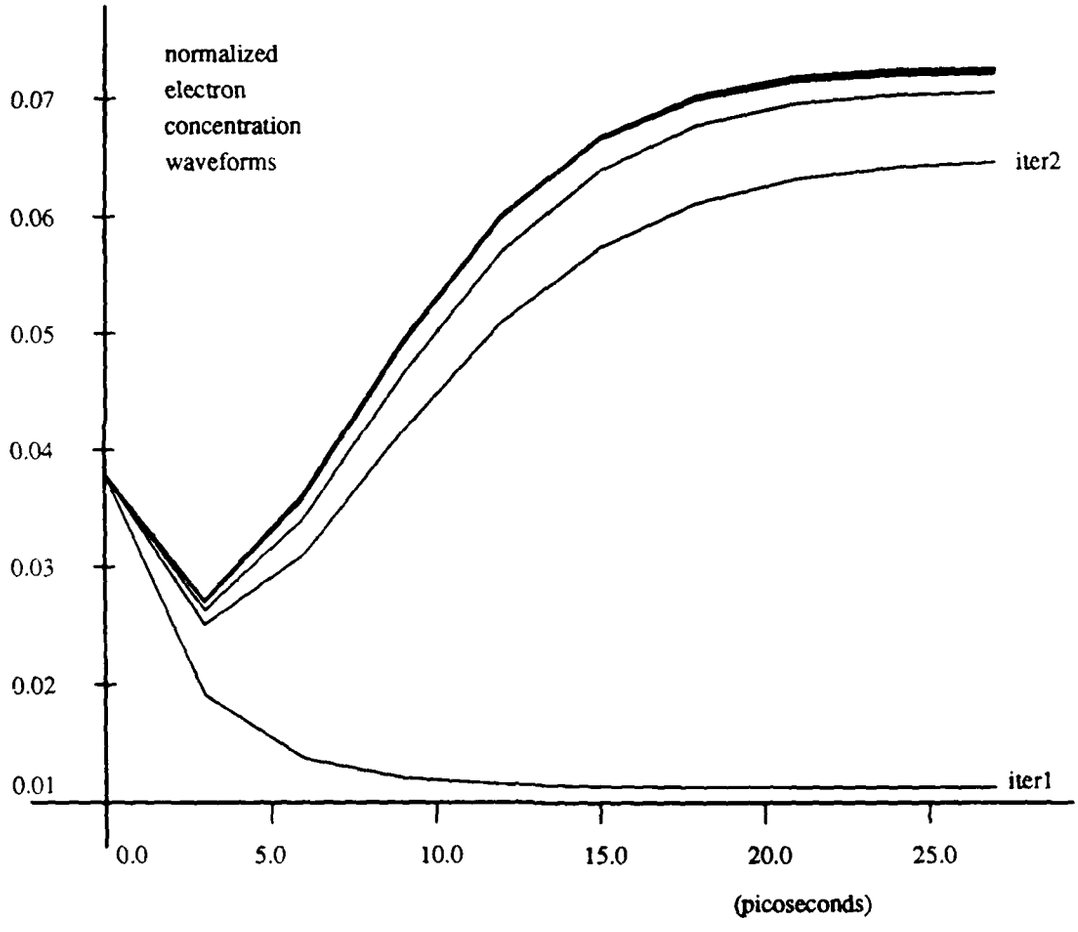

Figure 3: The waveforms converge uniformly, even when the timesteps are coarse.

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