

Adaptive Time Step Control for Semiconductor Simulations

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This paper presents an adaptive time-stepping strategy designed for semiconductor transient simulations. The strategy aims to minimize overall computational cost by balancing nonlinear iterations with local truncation error (LTE) estimation. In addition to LTE-based time-step control, the method dynamically adjusts time steps based on the convergence behavior of Newton iterations. Although the total number of time steps may slightly increase, the reduction in step size enhances Newton iteration convergence, resulting in lower overall computational overhead. The numerical results of semiconductor switching processes demonstrate that the strategy effectively captures sharp physical variations, reduces failed Newton iterations, and enhances overall computational efficiency.

Index Terms—adaptive time step control, drift-diffusion model, semiconductor device, transient simulation.

I. INTRODUCTION

DESIGN and optimization of semiconductor devices rely on accurate and efficient simulations [1]. In the classical drift-diffusion model, which neglects quantum effects, the physical processes within semiconductor devices are described by the following system of the Poisson and drift-diffusion equations [2]:

$$\epsilon \nabla^2 \psi = -q(p - n + N_D^+ - N_A^-), \quad (1)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot (-q\mu_n n \nabla \psi + qD_n \nabla n) + G_n - R_n, \quad (2)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot (-q\mu_p p \nabla \psi - qD_p \nabla p) + G_p - R_p, \quad (3)$$

where n , p and ψ represent the electron density, hole density, and electrostatic potential in the semiconductor, respectively; μ_n , μ_p , D_n , and D_p describe the mobilities and diffusion coefficients of electrons and holes, respectively. The parameters ϵ and q represent the dielectric permittivity of the medium and the elementary charge, respectively. The terms N_D^+ (resp. N_A^-) indicate the ionized donor (resp. acceptor) impurity concentrations. Additionally, G_i , R_i ($i = n, p$) signify the net generation and recombination rates of charge carriers.

In the transient simulation of semiconductor switching, capturing fast (nanosecond-scale) dynamics while minimizing computational resources for slower (microsecond-scale) processes is crucial. Existing adaptive time-stepping methods [3], while reducing the number of time steps, may overlook potential Newton iteration failures when larger steps are taken, thereby increasing computational costs.

To address these challenges, we propose integrating Newton convergence feedback into the classical LTE time step control framework. Numerical results demonstrate that this approach significantly reduces Newton iteration failures, thereby enhancing the overall computational efficiency of the simulations.

II. ADAPTIVE TIME STEP CONTROL STRATEGY

We use the Newton iterative convergence behavioral criterion to enhance the LTE-based time-step control. In this strategy, the time step achieves LTE-based adjustment only when the number of consecutive Newton iteration convergences

(denoted as N_{cc}) reaches a predefined threshold (denoted as N_{fix}). Otherwise, the step size remains frozen (i.e., non-growing). This increases the number of successful Newton convergences and improves computational efficiency.

Algorithm 1 Adaptive Time Step Algorithm

Ensure: Adaptive time-stepping solution x^{t_n} until $t_n = T$

- 1: **Initialize:** $n \leftarrow 0$, $t_n \leftarrow 0$, $h_n \leftarrow h_0$, $N_{cc} \leftarrow 0$, $h_{ratio} \leftarrow 1$
- 2: **while** $t_n < T$ **do**
- 3: **if** $t_n + h_n \geq T$ **then**
- 4: $h_n \leftarrow T - t_n$ ▷ Adjust step size to exactly reach T
- 5: **end if**
- 6: **Solve** $F(x^{n+1}) = 0$ using Newton's Method
- 7: **if** Newton's method converges **then**
- 8: $N_{cc} \leftarrow N_{cc} + 1$
- 9: Compute local truncation error (LTE)
- 10: **if** LTE satisfies tol requirements (see 4) **then**
- 11: **Accept** x^{n+1} and h_n
- 12: $h_{n+1} \leftarrow Q(h_n, r, h_{ratio})$
- 13: **if** $N_{cc} \leq N_{fix}$ **then**
- 14: $h_{ratio} \leftarrow 1$ ▷ frozen step size adjustment
- 15: **else**
- 16: $N_{cc} \leftarrow \max(N_{fix} - 1, 0)$, $h_{ratio} \leftarrow 2$
- 17: **end if**
- 18: $n \leftarrow n + 1$
- 19: **else**
- 20: **Reject** x^{n+1} and h_n
- 21: $h_n \leftarrow R(h_n)$
- 22: **if** $N_{cc} \leq N_{fix}$ **then**
- 23: $h_{ratio} \leftarrow 1$ ▷ frozen step size adjustment
- 24: **else**
- 25: $N_{cc} \leftarrow \max(N_{fix} - 1, 0)$, $h_{ratio} \leftarrow 2$
- 26: **end if**
- 27: **end if**
- 28: **else**
- 29: **Reject** x^{n+1} and h_n
- 30: $h_n \leftarrow \frac{1}{2} h_n$
- 31: $N_{cc} \leftarrow 0$, $h_{ratio} \leftarrow 1$
- 32: **end if**
- 33: **end while**
- 34: **return** Final solution $x(T)$

Consider the nonlinear ODE system resulting from spatial discretization, represented as $x'(t) = f(x, t)$. The workflow to compute x at a target time T is detailed in Algorithm 1, where t_n , h_n , and x^n denote the n -th time step, its size, and the solution at t_n , respectively. In this implementation, time discretization is performed using the TR-BDF2 method, which offers enhanced stability. As a single-step, second-order method, its LTE is given by: $LTE = \frac{(3\gamma^2 - 4\gamma + 2)}{6(\gamma - 1)} \tau h$, where

$\tau = \left[\frac{f(t_n)}{\gamma} - \frac{f(t_n + \gamma h)}{\gamma(1-\gamma)} + \frac{f'(t_n + h)}{1-\gamma} \right]$, $\gamma = 2 - \sqrt{2}$. The LTE criterion with the specified tolerance is determined by:

$$r = \sqrt{\frac{1}{N} \sum \left(\frac{\text{LTE}}{\varepsilon_r |x| + \varepsilon_a} \right)^2} < 2, \quad r_{\text{LE}} = r^{-\frac{1}{3}}, \quad (4)$$

where ε_r and ε_a are the user-specified relative and absolute error tolerances, respectively. If the condition (4) is not satisfied, the current step size is updated as $R(h_n) = 0.9 \cdot r_{\text{LE}} h_n$, otherwise, $Q = \min(r_{\text{LE}} h_n, h_{\text{ratio}} h_n, h_{\text{max}})$, where h_{max} represents the maximum allowable step size, while h_{ratio} is a step control ratio. In this study, we set $h_{\text{ratio}} \in \{1, 2\}$ and $\varepsilon_r = \varepsilon_a = 10^{-2}$.

III. APPLICATION AND RESULTS

We conducted a transient simulation experiment on the reverse-blocking IGCT (RB-IGCT)[4], with the standard test circuit and device doping structure illustrated in Fig. 1. Detailed circuit parameters can be found in [5].

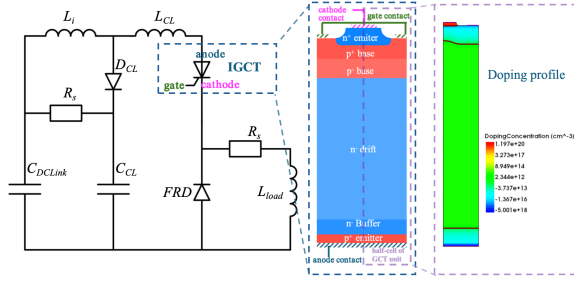


Fig. 1. Test circuit with a RB-IGCT and the device doping structure

For spatial discretization, we employ the FVSG method. The Dirichlet boundary conditions at the electrode interfaces are determined by solving the circuit equations using a two-level device-circuit iterative approach.

A. Accuracy validation

In this subsection, the proposed stepping strategy is validated by comparing the consistency of the transient waveforms of different methods. The voltage and current transients with ($N_{\text{fix}} = 2$) and without frozen time step process are shown in Fig. 2. The results accurately capture the turn-on and turn-off states of the RB-IGCT.

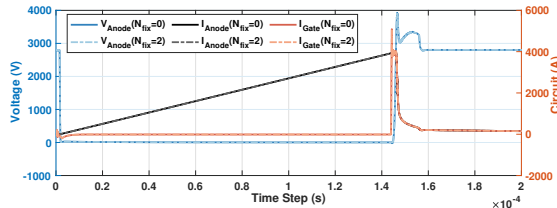


Fig. 2. Simulated transients during the Turn-on/Turn-off of RB-IGCT.

B. Efficiency comparison

To evaluate the computational efficiency of the proposed time-stepping strategy, we conducted a series of tests by adjusting the maximum allowed Newton iteration freezes, N_{fix} . The results include the total computation time, the counts of successful and failed Newton iterations, and the counts of successful and failed time steps, as shown in Fig. 3. To ensure

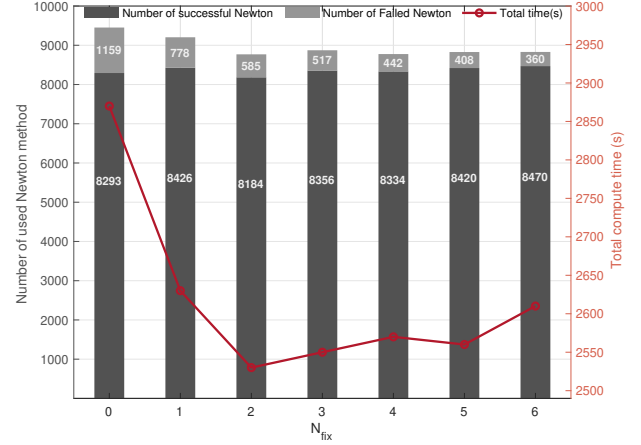


Fig. 3. Impact of N_{fix} on Newton iteration performance, and total computational time for the RB-IGCT transient simulation

reliability, the data represents the average of three experiments conducted under the same setup.

The results indicate that, compared to the method without Newton iteration control ($N_{\text{fix}} = 0$), introducing the Newton frozen time step strategy significantly improves the computational efficiency, even though the total number of time steps increases. Specifically, when $N_{\text{fix}} = 2$, computational efficiency improves by approximately 12.46% from 2890 s ($N_{\text{fix}} = 0$) to 2530 s, primarily due to the significant reduction in failed Newton iterations. This demonstrates that a proper choice of N_{fix} can balance the number of time steps and Newton iteration convergence, effectively reducing overall computational costs.

IV. CONCLUSION

Numerical experiments demonstrate that the proposed adaptive time-stepping strategy effectively reduces overall computational cost by optimizing Newton iteration performance, while slightly increasing the total number of time steps. Further implementation details and extended numerical results will be provided in a subsequent full version of this work.

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