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A Spectral Method for the Numerical Simulation of Transit-Time Devices

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Abstract

For the numerical simulation of semiconductor devices driven by a periodic voltage a new numerical approach is presented. The method is based on a temporal Fourier expansion to solve time-dependent nonlinear partial differential equations like the Drift-Diffusion Model. Disadvantages and problems of conventionally used time discretizations are avoided. To achieve high-accuracy results an interval based error-analysis is presented.

1. Introduction

The simulation of semiconductor devices with a periodic driven voltage requires the numerical solution of nonlinear partial differential equations. An often used model is the Drift-Diffusion Model (DDM). Typical applications are the simulation of IMPATT-, PIN- or BARITT-diodes, [1]. The usual way to approximate time derivatives is the discretization via Finite Differences. To obtain the periodic solution a decoupled one-step iteration is necessary, [2]. Besides of many required iteration cycles all known problems of Finite Difference Methods like low-order discretization are occuring. In order to avoid these problems a new method, the so-called t-Fourier Method (tFM), is presented here. Most theoretical aspects are common to the $\vec{x}$-Fourier Method [3]. With the formulated tFM all usual semiconductor equations describing time and space dependent transport phenomena of electrons and holes can be treated. For simplicity all subsequent details are performed for the DDM. For derivation, parameter selection and boundary values see [4]. The DDM can be written in the following manner

$$\frac{\partial}{\partial t}\begin{pmatrix} 0 \\ u_2 \\ u_3 \end{pmatrix} + F(u, \nabla u, \Delta u) \;=\; 0, \quad u = (u_1, u_2, u_3)^T \tag{1}$$

involving Poisson equation and continuity equations for electrons n and holes p. The electrostatic potential $u_1 = \varphi$ is determined at the contacts by the applied sinusoidal voltage $U(t) = U_0 + U_1 \sin(\omega t)$.

2. t-Fourier Method

The method presented is based on a temporal Fourier expansion of the solution vector

$$u(\vec{x},t) \;=\; \sum_{k=-\infty}^{\infty} \hat{u}_k(\vec{x}) e^{-ik\omega t} \tag{2}$$

This approach fullfills the periodicity condition automatically. Inserting (2) into the semiconductor equations (1) and applying the inner product $< .,. >$ of the underlying Sobolev-space the equations are transformed to an infinite system of nonlinear differential equations for the space dependent Fourier coefficients $\hat{u}_k$. This can easily be seen by utilizing the main features of spectral series like linearity, convolution, and transformation of time-derivatives into algebraic terms. The Fourier Spectrum of the nonlinear transcendental functions $\mu_{n,p}, G, R$ can be calculated in t-space.

Boundary conditions have to be transformed analogously. Thus, we obtain the Fourier-Galerkin coefficients $F_k := < F, e^{-ik\omega t} >, \; k = -\infty, ..., \infty$ of the basic operator F. A solution vector $(\hat{u}_k)_{k=-\infty,...,\infty}$ now has to fullfill the following equations:

$$G_k := -ik\omega(0, \hat{u}_{2k}, \hat{u}_{3k})^T + F_k \;=\; 0, \quad k = -\infty, ...\infty \tag{3}$$

3. Numerical Solution Procedure

For numerical treatment the infinite sum (2) is approximated by the M-th partial Fourier sum ($k = -M, ..., M$). Transcendental functions are calculated in t-space transformed with efficient FFT-techniques. Hence, one ends up solving a finite nonlinear system of differential equations. They can be discretized with well-known techniques like the Finite Element, Finite Difference or $\vec{x}$-Fourier Method. This leads to an algebraic nonlinear system G^M which is solvable with an efficient Newton algorithm:

$$u_0 \;:=\; (\tilde{u}_k, k = -M, ..., M) \tag{4}$$

$$u_{j+1} \;:=\; u_j - (\frac{dG^M}{du}(u_j))^{-1} G^M(u_j), \quad j > 0 \tag{5}$$

The Jacobian matrix dG^M/du depends on the $\vec{x}$-discretization used. The examples illustrated below were calculated with a classical Scharfetter-Gummel scheme which leads to a tridiagonal block matrix.

4. Examples

Some results for a Si-IMPATT diode are presented. The diode has a $N_D^+ N_D N_A N_A^+$ geometry (double drift) with $N_D = 10^{17}$ 1/cm^3 (300 nm), $N_A = 1.25 \cdot 10^{17}$ 1/cm^3 (300nm). The contacts were chosen to $N_D^+ = N_A^+ = 10^{18}$ 1/cm^3. For simplicity external circuits are neglected and the DDM is used in an one-dimensional formulation. Fig.1-3 show the electric field E and the electron and hole concentration n and p at the 4 significant time-points $t_1 = 0, t_2 = T/4, t_3 = T/2, t_4 = 3T/4, T = 2\pi/\omega$. The parameters were chosen to $U_0 = 24\text{V}, U_1 = 10\text{V}, f = 1/T = 60\text{GHz}, J_{DC} = 28.4\text{kA}/cm^2$. The solid line represents the solution with $M = 32$, dots $M = 10$. The results illustrate the very fast convergency of the Fourier coefficients. The tFM is unconditionally

stable. The Newton algorithm requires only few iterations and no damping technique.

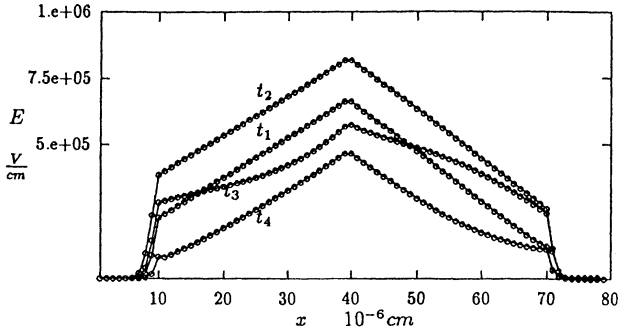

Figure 1: Electric Field $E(x, t_j)$

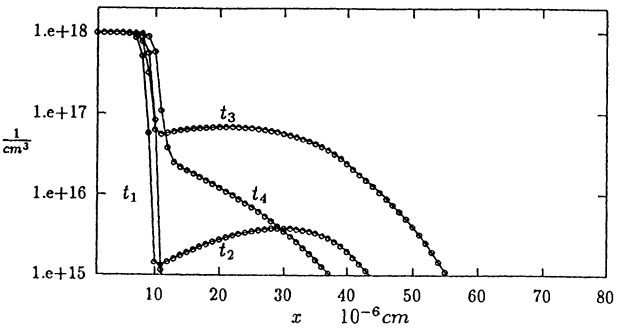

Figure 2: Electrons $n(x, t_j)$

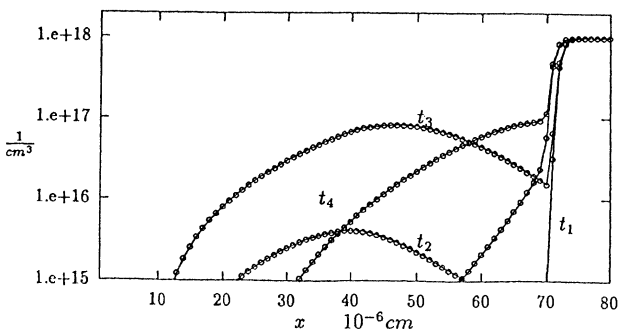

Figure 3: Holes $p(x, t_j)$

5. Interval based Error Control

The main advantage of Spectral Methods is the theoretical representation of the solution up to a very high accuracy. In the case of the semiconductor equations

this attribute is impaired by rounding and transformation error when treating the transcendental functions. An easy way to control these errors is the usage of Intervals [5]. During the application of the tFM equations of the form

$$f_k = \frac{1}{T}\int_0^T f(\sum_{j=-M}^{M} a_k e^{-ij\omega t})e^{ik\omega t}dt \tag{6}$$

with known a_k and f have to be solved. The coefficients f_k are calculated numerically via FFT-techniques. Rounding and transformation error can lead to unpredictable results. With XSC-Computer languages, e.g. [6], an error-control with intervals can easily be implemented. A practicable formula for a first error control is given with

$$R := f([0,T]) - \sum_{k=-M}^{M} \widetilde{f_k} e^{-ik\omega[0,T]} \tag{7}$$

The error of the numerically calculated Fourier coefficients $\widetilde{f_k}$ and the exact ones lie between bounds given by R for every k. For more sophisticated interval methods the reader is referred to later papers. A future step in error control will also be the calculation of verified results of the nonlinear algebraic system (3) with an Interval-Newton algorithm to prove the uniqueness and existence of a solution within narrow interval bounds, [7].

6. Conclusion

It has been proven that solving the time-periodic DDM with the tFM has many advantages in contrast to conventionally used time-discretizations. In addition to the efficient Newton algorithm the main feature is the avoidance of instabilities and diffusion problems. The most impressive result is the very low number of Fourier coefficients required to represent the solution with sufficient accuracy. With the posibilities of interval computation in error analysis Spectral Methods can lead to a new dimension in accuracy. Hence, the tFM is also an interesting alternative in the transient case.

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