Suppression of numerically induced chaos with nonstandard finite difference schemes

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Abstract

It has been previously shown that despite its simplicity, appropriate nonstandard schemes greatly improve or eliminate numerical instabilities. In this work we construct several standard and nonstandard finite-difference schemes to solve a system of three ordinary nonlinear differential equations that models photoconductivity in semiconductors and for which it has been shown that integration with a conventional fourth-order Runge–Kutta algorithm produces numerical-induced chaos. It was found that a simple nonstandard forward Euler scheme successfully eliminates these numerical instabilities. In order to help determine the best finite-difference scheme, it was found useful to test the local stability of the scheme by direct inspection of the eigenvalues dependent on the step size. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Conventional numerical techniques, such as the forward Euler and higher-order Runge–Kutta schemes, are extensively used in solving systems of nonlinear differential equations. However, these numerical procedures may lead to chaotic or spurious solutions which are strongly scheme dependent [1,2,14].

The present work specifically addresses the use of simple nonstandard numerical schemes [5] to overcome numerically induced chaos. Despite the availability of more sophisticated schemes, we

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are encouraged to use these simple techniques mainly because nonstandard schemes provide direct and easy to implement successful schemes, as found earlier [5–7]. In addition, commonly used or even advanced algorithms include at some level very basic standard constructions and it is precisely at this fundamental level where (chaotic) numerical instabilities could emerge. Therefore, simple nonstandard schemes may be potentially valuable in replacing these standard blocks within far more advanced schemes. For this purpose, we will investigate a nonlinear set of differential equations that model the photoconducting process of intrinsic semiconductors for which it was previously shown that the observed numerical chaotic behavior was a direct result of the integration scheme used [10,11]. These equations conform a relevant model of a more general character, because although here they describe the kinetics of charge carriers, the model is flexible enough to easily represent the dynamics of generation, trapping and annihilation between competing species. In this study, we employ the forward-Euler and central difference nonstandard schemes where nonlocal representations are made for the nonderivative terms and a denominator function is used to replace the step-size \( \Delta t = h \). For purposes of comparison, the standard versions of these schemes are also studied. In all cases, we choose or discard schemes by direct inspection of the stability properties of the resulting discrete models through the magnitude of the eigenvalues as a function of the step size.

2. The photoconductor model

The kinetics of charge carriers in intrinsic semiconductors has a complex behavior, particularly when photoconductivity is dominated by the presence of one or several types of traps and/or recombination centers caused by impurities or defects in the material. The resulting rate equations are nonlinear and since analytic solutions are difficult to obtain, numerical methods are necessarily used. For the case of one type of trap close enough to the conduction band such as to ensure thermally ejected electrons, the photoconducting process is described by the following set of nonlinear, coupled differential equations:

\[
\frac{dn}{dt} = G - n\varepsilon_1(N_t - m) + \gamma_1 m - c_1 n, \quad (1a)
\]

\[
\frac{dm}{dt} = n\varepsilon_1(N_t - m) - \delta_0 m p - \gamma_1 m, \quad (1b)
\]

\[
\frac{dp}{dt} = G - \delta_0 m p - c_2 p, \quad (1c)
\]

where \( n, m, \) and \( p \) represent, respectively, the electron, trapped electron, and hole population densities. The seven parameters take the values employed in Refs. [10,11]. These values are \( G = 10^6 \) electron–hole pairs/cm\(^3\) s, \( \varepsilon_1 = 4.1 \times 10^{-14} \) cm\(^3\) s\(^{-1}\), \( N_t = 10^{14} \) cm\(^{-3}\), \( c_1 = 1.5 \times 10^{-3} \) s\(^{-1}\), \( c_2 = 1.5 \times 10^{-5} \) s\(^{-1}\), \( \delta_0 = 10^{-15} \) cm\(^3\) s\(^{-1}\), and \( \gamma_1 = 0.83 \) s\(^{-1}\). The corresponding initial conditions are taken to be \( n_0 = 3 \times 10^{15} \) cm\(^{-3}\), \( m_0 = 10^{10} \) cm\(^{-3}\), and \( p_0 = 5 \times 10^{13} \) cm\(^{-3}\). For these values, the system becomes very stiff due to the very different time scales of the charge populations. For this situation, numerical solution of Eqs. (1a)–(1c) with a fixed step fourth-order Runge–Kutta (RK) scheme produced a remarkable output as shown in Fig. 1. Moreover, due to the nonlinear structure of system (1), a chaotic solution might be expected for this system, as observed in Fig. 1. However, in Refs. [10,11] it was shown...
that the onset and later collapse of the chaotic time series was an artifact of the particular numerical integration procedure, specifically the RK scheme. In fact, adaptive integration techniques appropriate for a stiff system, such as the Gear or Moulton–Adams schemes, promptly removed the complex behavior shown in Fig. 1, yielding smooth well-behaved curves.

As discussed in Refs. [10–12], the origin of the intermittent chaotic transient and the reverse period-doubling breakdown, shown in Fig. 1, was the formation of a nonlinear iterative structure arising from the RK algorithm which was capable of generating chaos. It has been found [1,2,14] that for step-sizes larger than some threshold value, the RK scheme becomes unstable and a numerical instability is manifested by the creation of additional real-valued spurious fixed points. In the case that these additional solutions may become chaotic, as is the situation for the photoconductor model, this type of instability could be regarded as a chaotic numerical instability [10–12].

We now construct a forward Euler nonstandard finite-difference scheme for the photo-conductor rate equations (1). Our particular nonstandard representation is

\[
\begin{align*}
\frac{n_{k+1} - n_k}{\phi(h)} &= G - (\varepsilon_1 N) n_{k+1} + \varepsilon_1 n_k m_k + \gamma_1 m_k - c_1 n_{k+1}, \\
\frac{m_{k+1} - m_k}{\phi(h)} &= (\varepsilon_1 N) n_k - \varepsilon_1 n_k m_{k+1} - \delta_0 m_{k+1} p_k - \gamma_1 m_{k+1}, \\
\frac{p_{k+1} - p_k}{\phi(h)} &= G - \delta_0 m_k p_{k+1} - c_2 p_{k+1},
\end{align*}
\]

where \(\phi(h)\) is a denominator function [5] that satisfies \(\phi(h) \to h + O(h^2)\) when \(h \to 0\). The above particular nonstandard scheme was selected so that positive values for \((n_k, m_k, p_k)\) imply positive values for \((n_{k+1}, m_{k+1}, p_{k+1})\). This requirement follows from the physical property that \((n, m, p)\) are particle densities and, consequently, by definition are nonnegative. Any finite-difference scheme that allows negative solutions will have numerical instabilities. It is simple to see that other possible choices of substitutions for the nonderivative terms could lead to negative solutions for the discrete equations. For example, this might occur if a term like \(\delta_0 mp\) in Eq. (1c) is replaced by \(\delta_0 m_k p_k\) instead of \(\delta_0 m_k p_{k+1}\) in Eq. (2c).
For the same parameter values and initial conditions employed in Refs. [10,11], the nonstandard forward Euler (NSFE) representation Eqs. (2a)–(2c) was solved using the following denominator function [5,6]:

$$\phi(h) = T \left[ 1 - \exp \left( -\frac{h}{T} \right) \right],$$

where $T$ is the smallest time scale occurring in the photoconductor system. For the parameters used in this paper, $T$ was selected to be $T = \gamma_1^{-1}$. Note that for any finite positive step-size, $\phi(h)$ is always bounded above by $T$, i.e., $0 < \phi(h) < T$. Results are shown in Fig. 2 for the electron population and coincides with the curves previously obtained by the adaptive Gear integration method in Ref. [10]: that is, all chaotic behavior has disappeared and the fixed points of Eqs. (2a)–(2c) are exactly the same equilibrium points obtained for the photoconductor system differential equations.

For purposes of comparison, we also constructed a finite difference model of Eqs. (1a)–(1c) according to a standard forward Euler (SFE) representation: the conventional calculus definition [4] for the first derivative and the usual direct substitutions for the nonderivative terms. In explicit form, the SFE scheme is given as

$$n_{k+1} = n_k [1 - \phi(x_1N_k - x_1 m_k + c_1)] + \phi (G + \gamma_1 m_k),$$

$$m_{k+1} = m_k [1 - \phi(x_1 n_k + \delta_0 p_k + \gamma_1)] + \phi x_1 N_k n_k,$$

$$p_{k+1} = p_k [1 - \phi(\delta_0 m_k + c_2)] + \phi G,$$

where $\phi(h)$ will be taken as either that given in Eq. (3) or the standard choice $\phi(h) = h$. The fixed points for this scheme have the same values as the equilibrium points of Eqs. (1a)–(1c). However, implementation of the SFE scheme produced numerical overflow for all step sizes.

Similar results were obtained by constructing a finite difference scheme for Eqs. (1a)–(1c) based on a standard central difference scheme (SCD), where the first derivative is substituted by the general form

$$\frac{dy}{dt} \rightarrow \frac{y_{k+1} - y_{k-1}}{2h}$$

Fig. 2. Solution for the electron population according to a forward-Euler nonstandard scheme for the same parameters as in Fig. 1.
and with the same local substitutions as used for the SFE construction. Solving Eqs. (1a)–(1c) by this SCD scheme produced numerical overflow for all values of the integration step size. The use of a central difference (CD) scheme for Eqs. (1a)–(1c) certainly leads to numerical instabilities [5], as the order of this type of scheme is greater than the order of the photoconductor differential equations. This situation has been extensively studied in scalar nonlinear differential equations [5,13]. In particular, Yamaguti and Ushiky [13] showed that a CD scheme can induce numerical chaos because of the emergence of homoclinic orbits. This particular origin for numerical chaos was also indicated as a cause for the chaotic behavior in Refs. [11,12]. Furthermore, like the CD scheme, the order of the Runge–Kutta scheme used for solving the photoconductor model [10,11] is greater than the order of the differential Eq. (1). Therefore, numerical instabilities for a threshold step size were expected and found [10,11].

A nonstandard central difference (NSCD) representation of Eq. (1) is given by

\[
\frac{n_{k+1} - n_{k-1}}{2\phi(h)} = G - n_{k+1} z_1 N_t + n_k z_1 m_k + \gamma_1 m_k - c_1 n_{k+1},
\]

\[
\frac{m_{k+1} - m_{k-1}}{2\phi(h)} = n_k z_1 N_t - n_k z_1 m_{k+1} - \delta_0 m_{k+1} p_k - \gamma_1 m_{k+1},
\]

\[
\frac{p_{k+1} - p_{k-1}}{2\phi(h)} = G - \delta_0 m_k p_{k+1} - c_2 p_{k+1},
\]

where the nonlocal representations of Eqs. (2a)–(2c) are used and \(\phi(h)\) is the denominator function. Interestingly, solving Eqs. (1) with the nonstandard CD scheme Eqs. (6a)–(6c) lead to overflow as the standard CD, but only after a finite number of iterations, depending on the value of the step size. Fig. 3 shows this dependence and it is possible to observe that for a sufficient small step size no overflow seems to occur for an a priori given number of iterations. Thus, despite the restrictions imposed on the magnitude of the step-size, the nonlocal substitutions made for the nonderivative terms of Eqs. (1a)–(1c) produced an improvement relative to the stability properties of the SCD scheme.
In the following section, it will be shown that the same conclusions, obtained so far through direct numerical integration of the SFE, NSFE, SCD, and NSCD schemes, can be easily and quickly reached by direct examination of the eigenvalues from the finite difference equations.

3. Stability analysis

The photoconductor system has two fixed points, one of which has negative values for the charge densities \((n, m, p)\) and thus has no physical meaning. The other fixed point gives positive values for the charge densities and the stability analysis is made for this case, and is given by \(n = 3.44 \times 10^{15}\) cm\(^{-3}\), \(m = 2.90 \times 10^{13}\) cm\(^{-3}\), and \(p = 3.44 \times 10^{17}\) cm\(^{-3}\). The eigenvalues associated with a linear stability analysis are calculated by solving the equation \(\det(J - \lambda I) = 0\), where \(J\) is the Jacobian of the system Eq. (1) evaluated at the equilibrium and \(I\) is the identity matrix. The real parts of the resulting eigenvalues are negative: \(\lambda_1 = -0.0000209\), \(\lambda_2 = -487.18\), \(\lambda_3 = -2.066\). Consequently, the equilibrium point for Eqs. (1a)–(1c) is locally stable [3,9]. Alternatively, one can use the Routh–Hurwitz criterion for stability [3] to show that the fixed point of Eq. (1) is linearly stable if \(N_t > \tilde{m}\). With our parameter values, this result holds true. Therefore, an appropriate finite difference integration scheme for solving the photoconductor model should yield the same fixed point with this stability feature, otherwise, the scheme is numerical unstable.

The NSFE scheme, given by Eqs. (2a)–(2c), can be rewritten to the explicit form

\[
n_{k+1} = \frac{\phi G + n_k (1 + \phi z_1 m_k) + \phi \gamma_3 m_k}{1 + \phi (z_1 N_t + c_1)}, \tag{7a}
\]

\[
m_{k+1} = \frac{m_k + \phi z_1 N_t n_k}{1 + \phi (z_1 n_k + \delta_0 p_k + \gamma_1)}. \tag{7b}
\]

\[
p_{k+1} = \frac{\phi G + p_k}{1 + \phi (\delta_0 m_k + c_2)}. \tag{7c}
\]

The fixed points of Eqs. (7a)–(7c) are obtained by solving these equations under the conditions \(n_{k+1} = n_k\), \(m_{k+1} = m_k\), and \(p_{k+1} = p_k\). An easy calculation shows that Eqs. (7a)–(7c) have the exact same physical fixed point as the differential equation (1). The linear stability properties of this fixed point are determined by the eigenvalues of the Jacobian, \(J_k\), associated with Eqs. (7a)–(7c). Let \(F_1, F_2,\) and \(F_3\) be the right sides of, respectively Eqs. (7a), (7b), and (7c). Let \(F_{1n} \equiv \partial F_1 / \partial n_k\), etc., evaluated at \(n_k = \tilde{n}\), \(m_k = \tilde{m}\), and \(p_k = \tilde{p}\). The Jacobian of Eqs. (7a)–(7c) is given as

\[
J_k = \begin{pmatrix}
F_{1n} & F_{1m} & F_{1p} \\
F_{2n} & F_{2m} & F_{2p} \\
F_{3n} & F_{3m} & F_{3p}
\end{pmatrix}.
\tag{8}
\]

The discrete eigenvalues of \(J_k\) can be obtained by solving the equation \(\det(J_k - \lambda I) = 0\).

We find that for the NSFE scheme, the three eigenvalues satisfy the condition, \(|\lambda_i| < 1\) \((i=1,2,3)\), for all \(h > 0\). This implies that the fixed point, \(n_k = \tilde{n}\), \(m_k = \tilde{m}\), and \(p_k = \tilde{p}\), is linearly stable [8] as in the continuous-time system (1). Consequently, it can be concluded that the NSFE scheme is a good scheme for use in the numerical integration of the photoconductor differential equations. The stability analysis for the standard forward Euler (SFE) was also done. Using the same procedure
Fig. 4. The largest eigenvalue from a standard central difference construction of the photoconductor system solved with different denominator functions \( \phi(h) \). The saturated upper curve is for a denominator function as in equation (3), the decreasing lower curve is for the standard selection \( \phi(h) = h \). The magnitude of \( \lambda_1 \) is much larger than the corresponding eigenvalue from the NSCD scheme and the SFE scheme.

outlined for the NSFE scheme, a local stability analysis revealed that one eigenvalue is \( \lambda_1 > 1 \) regardless of the step size, differently from the eigenvalue behavior of (1). This is in agreement with the observed overflow found in the direct SFE integration of Eqs. (1a)–(1c). Therefore, the SFE approach produces numerical instabilities and thus is not an appropriate scheme for the stiff nonlinear photoconductor system of Eqs. (1a)–(1c). For the nonstandard central difference system (6), a similar analysis as for the NSFE case shows that there is always present at least one eigenvalue greater in magnitude than unity for all step sizes in accordance with the overflow obtained.

An important point to note is that the eigenvalues obtained from a finite-difference model of a set of differential equations are not only a function of the system parameters, but also depend on the step size even in the form of a denominator function (9), i.e., for our problem,

\[
\lambda = f(G, x_1, N_t, c_1, c_2, \delta_0, \gamma_1, \phi(h)).
\]  

From this perspective, it is possible to study the stability performance of a given finite difference construction of a differential equation not only by varying the step size \( h \), but also by directly seeing the effects of using different denominator functions. In Fig. 4, we compare the behavior of the largest eigenvalue, \( \lambda_1 \), for a standard CD scheme, for the case where \( \phi(h) \) is given by Eq. (3) and for the standard situation where \( \phi(h) = h \). The magnitude of the eigenvalue is much larger than those corresponding to the other schemes, which renders as useless a CD scheme, in accordance with Refs. [5,13]. However, this figure illustrates the remarkable effect when a nonstandard denominator function is used.

4. Conclusions

The use of a nonstandard forward Euler scheme [5] for the numerical integration of the coupled, nonlinear photoconductor differential equations produced a numerical stable and well behaved solution, despite the considerable stiffness of the system. This is in contrast to conventional schemes, such as the fourth-order Runge–Kutta algorithm, where chaos arising from the numerical scheme
has been clearly established [10,11]. The proper choice of the scheme and the nonlocal substitutions proved to be critical for the performance of the scheme. These issues were resolved by simply examining the dependence of the eigenvalues on the time step-size. Therefore, it is proposed that these simple nonstandard constructions may be incorporated advantageously in the fundamental basis of more advanced numerical integrators for ODEs.

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