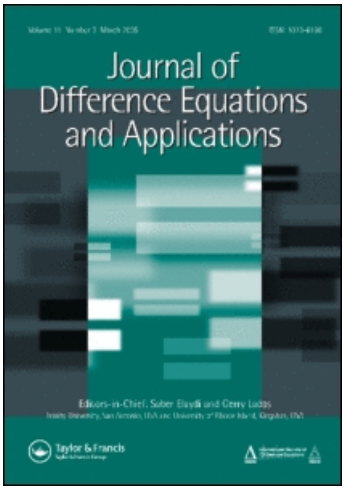

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Nonstandard Finite Difference Schemes for Differential Equations

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Nonstandard Finite Difference Schemes for Differential Equations

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This Paper is dedicated to Allan Peterson in celebration of his 60th birthday and for his many contributions to differential and difference equations.

This paper gives an introduction to nonstandard finite difference methods useful for the construction of discrete models of differential equations when numerical solutions are required. While the general rules for such schemes are not precisely known at the present time, several important criterion have been found. We provide an explanation of their significance and apply them to several model ordinary and partial differential equations. The paper ends with a discussion of several outstanding problems in this area and other related issues.

Keywords: Numerical analysis; Exact finite difference schemes; Numerical instabilities; Positivity; Difference equations

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INTRODUCTION

Few of the differential equations which provide mathematical models of important dynamical systems in the engineering and natural sciences can be solved exactly in terms of a finite number of the elementary functions [1]. Consequently, a variety of methods have been constructed to calculate numerical solutions. In particular, the use of finite difference procedures has played a significant role in this area [2–5]. However, a major difficulty is the occurrence of numerical instabilities [2,6]. In general, numerical instabilities are solutions to the discrete finite difference equations that do not correspond to any solution of the original differential equations. Examples of elementary forms of numerical instabilities include "ghost solutions" when the step-size is too large for ordinary differential equations [1,7], the change of linear stability properties of special solutions when the order of the difference equations is larger than that of the differential equations [7], and the creation of additional fixed-points [6,7]. Another source of numerical instabilities occurs when the discrete equations do not satisfy certain constraint conditions obeyed by the differential equations [8,9]. Such constraints include conservation of energy, monotonicity, boundedness, and positivity.

Almost all of the standard procedures yield schemes for which one or more of the above indicated difficulties arise. Our research program for the past decade has centered on the creation of new methods for constructing finite difference schemes such that these problems either do not occur or are minimized. We call these new procedures "nonstandard finite difference schemes" (NSFΔ). The general evolution of this topic can be found by examining the following Refs. [6,10,11].

The main purpose of this paper is to introduce the concept of NSFΔ schemes, state the most important rules for their construction, and illustrate their use by applying them to several well known differential equations.

The next section introduces the concept of an "exact finite difference scheme" for a differential equation. Based on investigations related to constructing exact schemes, the third section presents four fundamental rules used in the construction of NSFΔ schemes. The fourth section applies the rules to five nonlinear differential equations and briefly examines the influence of having the discrete models satisfy certain *a priori* desired constraints. Finally, in the last section, a general discussion is given on the

current status of NSFΔ schemes and several outstanding problems are presented.

EXACT FINITE DIFFERENCE SCHEMES

Consider a dynamical system described by a first-order scalar equation

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(u, t, \lambda), \quad u(t_0) = u_0, \tag{2.1}$$

where λ is the system parameters and $f(u, t, \lambda)$ is such that a unique solution exists for $t_0 \leq t < T$. (Note that for many dynamical systems modeling physical phenomena, $T = \infty$.) Let the solution to Eq. (2.1) be

$$u(t) = \phi(\lambda, u_0, t_0, t), \tag{2.2}$$

with

$$\phi(\lambda, u_0, t_0, t_0) = u_0. \tag{2.3}$$

Denote a finite difference model of Eq. (2.1)

$$u_{k+1} = F(\lambda, h, u_k, t_k), \tag{2.4}$$

where $h = \Delta t$, $t_k = hk$, and $u_k \approx u(t_k)$. Let the solution of Eq. (2.4) written in the form

$$u_k = \psi(\lambda, h, u_0, t_0, t_k), \tag{2.5a}$$

with

$$\psi(\lambda, h, u_0, t_0, t_0) = u_0. \tag{2.5b}$$

DEFINITION 2.1 Equations (2.1) and (2.4) are said to have the *same general solution* if and only if

$$u_k = u(t_k), \tag{2.6}$$

for $h > 0$.

DEFINITION 2.2 An *exact finite difference* scheme is one for which the solution of the difference equation has the *same general solution* as the associated differential equation.

THEOREM 2.1 *The first order differential equation*

$$\frac{du}{dt} = f(u, t, \lambda), \quad u(t_0) = u_0, \tag{2.7}$$

has an exact finite difference scheme given by

$$u_{k+1} = \phi(\lambda, u_k, t_k, t_{k+1}) \tag{2.8}$$

where the function ϕ is the same as that in Eq. (2.2).

Proof [6] The group property of the solutions to Eq. (2.7) gives [12]

$$u(t + h) = \phi[\lambda, u(t), t, t + h]. \tag{2.9}$$

Making the substitutions

$$t \rightarrow t_k, \quad u(t) \rightarrow u_k, \tag{2.10}$$

in Eq. (2.9) gives

$$u_{k+1} = \phi(\lambda, u_k, t_k, t_{k+h}), \tag{2.11}$$

which is a difference equation having the same general solution as Eq. (2.7). Thus, the result given by Eq. (2.11) is an exact scheme for Eq. (2.7). □

Note that this theorem can be directly generalized to systems of first-order differential equations. If the solutions to Eq. (2.7) exist for all time, i.e. $T = \infty$, then Eq. (2.8) holds for all t and h; otherwise, the relation is assumed to hold when the right-side of Eq. (2.11) is defined.

A major consequence of the theorem is that given a system of coupled, first-order ordinary differential equations, if the general solution is known, then an exact finite difference scheme can be constructed. However, for systems for which the general solution is unknown, the theorem provides no guidance as to what the exact scheme is. But, one can study the structure of exact schemes and examine the general observed properties to find hints as to how to make improved constructions for the finite difference schemes of differential equations. To date, this procedure has formed the basis of our research program on nonstandard schemes.

To illustrate the construction of exact schemes, consider the decay equation

$$\frac{du}{dt} = -\lambda u, \quad u(t_0) = u_0, \tag{2.12}$$

where the exact solution is

$$u(t) = u_0 \, \mathrm{e}^{-\lambda(t-t_0)}. \tag{2.13}$$

Applying the theorem, see the results in Eq. (2.10), we obtain for the exact scheme

$$u_{k+1} = u_k \, \mathrm{e}^{-\lambda h}, \tag{2.14}$$

which can be rewritten to the form

$$\frac{u_{k+1} - u_k}{\left(\frac{1-\mathrm{e}^{-\lambda h}}{\lambda}\right)} = -\lambda u_k. \tag{2.15}$$

This result is to be contrasted with the standard forward-Euler scheme

$$\frac{u_{k+1} - u_k}{h} = -\lambda u_k, \tag{2.16}$$

which is known to have numerical instabilities for $h \geq 1$ [6].

The logistic differential equation, in its general form, is

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \lambda_1 u - \lambda_2 u^2, \quad u(t_0) = u_0. \tag{2.17}$$

Its exact solution is

$$u(t) = \frac{\lambda_1 u_0}{(\lambda_1 - u_0\lambda_2)\exp[-\lambda_1(t - t_0)] + \lambda_2 u_0}. \tag{2.18}$$

Making in Eq. (2.18) the substitutions

$$t_0 \rightarrow t_k, \quad t \rightarrow t_{k+1}, \quad u_0 \rightarrow u_k, \quad u(t) \rightarrow u_{k+1}, \tag{2.19}$$

gives, after some rearranging, the exact finite difference scheme

$$\frac{u_{k+1} - u_k}{\left(\dfrac{\mathrm{e}^{-\lambda_1 h} - 1}{\lambda_1}\right)} = \lambda_1 u_k - \lambda_2 u_{k+1} u_k. \tag{2.20}$$

A somewhat more complicated situation occurs for two coupled, linear equations with constant coefficients, i.e.

$$\frac{\mathrm{d}u}{\mathrm{d}t} = au + bw, \quad \frac{\mathrm{d}w}{\mathrm{d}t} = cu + dw. \tag{2.21}$$

After a considerable number of algebraic manipulations, the following exact finite difference scheme is found

$$\frac{u_{k+1} - \psi u_k}{\phi} = a u_k + b w_k, \quad \frac{w_{k+1} - \psi w_k}{\phi} = c u_k + \mathrm{d} w_k, \tag{2.22}$$

where

$$\psi = \frac{\lambda_1 \, \mathrm{e}^{\lambda_2 h} - \lambda_2 \, \mathrm{e}^{\lambda_1 h}}{\lambda_1 - \lambda_2}, \quad \phi = \frac{\mathrm{e}^{\lambda_1 h} - \mathrm{e}^{\lambda_2 h}}{\lambda_1 - \lambda_2}, \tag{2.23}$$

and, λ_1 and λ_2 are solutions of the characteristic equation

$$\det \begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix} = 0. \tag{2.24}$$

In particular, the damped harmonic oscillator equation

$$\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} + 2\epsilon \frac{\mathrm{d}u}{\mathrm{d}t} + u = 0, \tag{2.25}$$

has the system equations

$$\frac{\mathrm{d}u}{\mathrm{d}t} = w, \quad \frac{\mathrm{d}w}{\mathrm{d}t} = -u - 2\epsilon w. \tag{2.26}$$

The corresponding exact finite difference scheme is

$$\frac{u_{k+1} - \psi u_k}{\phi} = w_k, \quad \frac{w_{k+1} - \psi w_k}{\phi} = -u_k - 2\epsilon w_k, \tag{2.27}$$

where

$$\psi = \frac{\epsilon \mathrm{e}^{-\epsilon h}}{\sqrt{1 - \epsilon^2}} + \mathrm{e}^{-\epsilon h} \cos\left(\sqrt{1 - \epsilon^2} h\right), \tag{2.28a}$$

$$\phi = \frac{\mathrm{e}^{-\epsilon h}}{\sqrt{1 - \epsilon^2}} \sin\left(\sqrt{1 - \epsilon^2} h\right). \tag{2.28b}$$

In the form of a second order difference equation, we have

$$\left[\frac{u_{k+1} - 2u_k + u_{k-1}}{\phi^2}\right] + 2\epsilon \left[\frac{u_k - \psi u_{k-1}}{\phi}\right] + \left[\frac{2(1 - \psi) u_k + (\phi^2 + \psi^2 - 1) u_{k-1}}{\phi^2}\right] = 0. \tag{2.29}$$

For partial differential equations having exact solutions, the procedure for obtaining exact finite difference schemes is somewhat modified from that required for ordinary differential equations. Consider the one-dimensional unidirectional wave equation with the initial value given over $-\infty < x < \infty$, i.e.

$$u_t + u_x = 0, \quad u(x,0) = f(x). \tag{2.30}$$

The solution to this problem is

$$u(x,t) = f(x-t). \tag{2.31}$$

Now the first order partial difference equation

$$u_m^{k+1} = u_{m-1}^k, \tag{2.32}$$

has as its general solution an arbitrary function of $(m-k)$ [13], i.e.

$$u_m^k = F(m-k). \tag{2.33}$$

If we select $\Delta x = \Delta t$, define $t_k = (\Delta t)k$ and $x_m = (\Delta x)m$, and set $u_m^k = u(x_m, t_k)$, then Eqs. (2.30) and (2.32) have the general solutions for the initial value problem. Consequently, Eq. (2.32) can be rewritten as

$$\frac{u_m^{k+1} - u_m^k}{\phi(\Delta \mathrm{x})} + \frac{u_m^k - u_{m-1}^k}{\phi(\Delta \mathrm{x})} = 0, \quad \Delta t = \Delta x, \tag{2.34}$$

where $\phi(z)$ is arbitrary, except for the condition

$$\phi(z) = z + O(z^2). \tag{2.35}$$

Observe that a functional relation exists between the space and time step-sizes. Likewise, the unidirectional wave equation having spherical symmetry is [14]

$$\frac{\partial u}{\partial t} + \frac{u}{r} + \frac{\partial u}{\partial r} = 0, \tag{2.36}$$

and the corresponding exact finite difference scheme is [14] for $u_m^k = u(x_m, r_k)$ the expression

$$\frac{u_m^{k+1} - u_m^k}{\Delta t} + \frac{u_{m-1}^k}{r_m} + \frac{u_m^k - u_{m-1}^k}{\Delta r} = 0, \quad \Delta t = \Delta r. \tag{2.37}$$

The addition of a nonlinear (logistic) reaction term, $u(1-u)$, to Eq. (2.30) produces the equation

$$u_t + u_x = u(1-u), \quad u(x,0) = f(x), \tag{2.38}$$

considered as an initial value problem where $f(x)$ is assumed to have a first derivative. The nonlinear transformation

$$u(x,t) = \frac{1}{w(x,t)}, \tag{2.39}$$

reduces Eq. (2.38) to the following linear, inhomogeneous equation

$$w_t + w_x = 1 - w, \tag{2.40}$$

which can be readily solved to give

$$w(x,t) = g(x-t)\mathrm{e}^{-t} + 1, \tag{2.41}$$

where $g(z)$ is arbitrary except for having a first derivative. Note that

$$g(x) = \frac{1-f(x)}{f(x)}, \tag{2.42}$$

thus

$$u(x,t) = \frac{f(x-t)}{\mathrm{e}^{-t} + (1-\mathrm{e}^{-t})f(x-t)}, \tag{2.43}$$

and

$$f(x-t) = \frac{\mathrm{e}^{-t}u(x,t)}{1-(1-\mathrm{e}^{-t})u(x,t)}. \tag{2.44}$$

Making the substitutions

$$x \rightarrow x_m, \quad t \rightarrow t_k, \quad u(x,t) \rightarrow u_m^k, \tag{2.45}$$

and using the fact that (see Eqs. (2.32) and (2.33))

$$f(x-t) \rightarrow f_m^k, \quad f_m^{k+1} = f_{m-1}^k, \tag{2.46}$$

it follows, after some algebraic manipulations, that the exact scheme for Eq. (2.38) is

$$\frac{u_m^{k+1} - u_m^k}{\phi(\Delta t)} + \frac{u_m^k - u_{m-1}^k}{\phi(\Delta x)} = u_{m-1}^k(1 - u_m^{k+1}), \tag{2.47}$$

where $\Delta x = \Delta t = h$, and

$$\phi(z) = e^z - 1. \tag{2.48}$$

Since this expression is linear in u_m^{k+1}, solving for it gives the explicit scheme

$$u_m^{k+1} = \frac{u_{m-1}^k}{1 + (e^h - 1)u_{m-1}^k}, \quad \Delta t = \Delta x. \tag{2.49}$$

Based on these and many other examples, we have formulated a basic set of modeling rules for constructing nonstandard schemes for differential equations. These rules are given in the next section along with a brief discussion of their practical significance.

RULES FOR CONSTRUCTING NONSTANDARD SCHEMES

A detailed study of Eqs. (2.15), (2.20), (2.27), and (2.47) shows that the discrete derivative generally takes on a form more complicated than the usual forward-Euler representation [2–5]. In fact, we have

$$\frac{du}{dt} \to \frac{u_{k+1} - \psi u_k}{\phi}, \tag{3.1}$$

where ψ and ϕ depend on the step-size $\Delta t = h$ and other parameters occurring in the differential equation, and, in addition, satisfies the conditions

$$\psi = 1 + O(h), \quad \phi = h + O(h^2). \tag{3.2}$$

The functions ψ and ϕ vary from one equation to another and, at this stage of the investigation, no clear *a priori* set of guidelines exist for determining them. However, for particular classes of equations, some progress has been made; see Refs. [15,16]. In most applications, ψ is usually selected to be $\psi = 1$, and ϕ (called the "denominator function") is determined by the requirement of having the correct stability properties for special solutions to the differential equations. The Refs. [15,16] show in detail how this can be achieved for the class of scalar ODE's

$$\frac{du}{dt} = f(u). \tag{3.3}$$

For these equations the nonstandard scheme is taken to be

$$\frac{u_{k+1} - u_k}{\phi} = f(u_k), \tag{3.4}$$

where ϕ is given by

$$\phi(h, R^*) = \frac{1 - \mathrm{e}^{-R^* h}}{R^*}. \tag{3.5}$$

The value of R^* is determined as follows. First, calculate the fixed-points of Eq. (3.3), i.e.

$$f(\bar{u}) = 0. \tag{3.6}$$

Assume that Eq. (3.6) has I-real solutions and denote them by $\{\bar{u}^{(i)};\ i = 1, 2, \ldots, I\}$. Now define R_i as

$$R_i \equiv \left.\frac{\mathrm{d}f}{\mathrm{d}u}\right|_{u=\bar{u}^{(i)}}, \tag{3.7}$$

and take R^* to be

$$R^* \equiv \max\{|R_i|; i = 1, 2, \ldots, I\}. \tag{3.8}$$

Note that $\phi(h, R^*)$ has the properties

$$\phi = h + O(R^* h^2), \quad 0 < \phi < \frac{1}{R^*}. \tag{3.9}$$

The result given in Eq. (3.5) can be given a physical interpretation which also leads to a fundamental understanding of what ϕ represents. Consider a dynamical system where the independent variable t is the time. It follows that the R_i have units of inverse time and a set of time scales can be defined by means of the relations

$$T_i \equiv \frac{1}{R_i}, \quad i = 1, 2, \ldots, I; \quad T^* = \frac{1}{R^*}. \tag{3.10}$$

Thus, T^* corresponds to the smallest time scale and a simple calculation shows that

$$0 < \phi(h, T^*) < T^*. \tag{3.11}$$

Consequently, the function ϕ can be interpreted as a "renormalized" or "rescaled" time step-size such that its value is never larger than the smallest time scale of the system. Since many of the mechanisms that lead to the occurrence of numerical instabilities have their origin in using a step-size that is greater than some relevant physical time scale, this method for selecting ϕ eliminates these type of instabilities. In other words, the use of the function ϕ, rather than just h, in Eq. (3.4), allows the value of h to be much larger than one normally selected because it is the effective step-size ϕ that determines the stability and not the actual step-size h.

Another issue of great importance is that in general nonlinear terms are modeled by discrete expressions that are nonlocal on the computational grid. For example, the u^2 term in the logistic equation (2.17) is replaced by $u_{k+1}u_k$ in the exact finite difference scheme, whereas conventional methods would use the local form $(u_k)^2$. A similar situation holds for the unidirectional wave equation (2.38) and its exact scheme given in Eq. (2.47) is

$$u^2 \rightarrow u_{m-1}^k u_m^{k+1}. \tag{3.12}$$

Note that each factor of u is evaluated at a different discrete space and time variables.

Based on these and other related results, the following rules for constructing nonstandard schemes for differential equations have been selected. The details behind these rules, as well as the required explanations as to how they were derived, are given in Ref. [11], Chapter 1; also, see Ref. [6].

Rule 1. The orders of the discrete derivatives should be equal to the orders of the corresponding derivatives of the differential equations.

Comment 1. If the orders of the discrete derivatives are larger than those occurring in the differential equations, then spurious solutions (numerical instabilities) will occur [2,6].

Rule 2. Discrete representations for derivatives must, in general, have nontrivial denominator functions.

Comment 2. The discrete first derivative, for example, takes the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} \rightarrow \frac{u_{k+1} - u_k}{\phi}, \tag{3.13}$$

where ψ and ϕ have the properties given by Eq. (3.2). This result can be generalized to both partial and higher-order derivatives.

Rule 3. Nonlinear terms should, in general, be replaced by nonlocal discrete representations.

Comment 3. For the logistic differential equation the u^2 term was replaced by $u_{k+1}u_k$. However, sometimes more general forms may be required, such as

$$u^2 = 2u^2 - u^2 \rightarrow 2(u_k)^2 - u_{k+1}u_k. \tag{3.14}$$

Rule 4. Special conditions that hold for the solutions of the differential equations should also hold for the solutions of the finite difference scheme.

Comment 4. Numerical instabilities can occur when the finite difference equations do not satisfy a condition that is of importance for the corresponding differential equations. For example, for many dynamical systems a condition of positivity holds for the dependent variables. If the numerical scheme leads to solutions that can violate this condition, then numerical instabilities will eliminate any possibility of obtaining meaningful numerical results.

A nonstandard finite difference scheme is any discrete representation of a system of differential equations that is constructed according to the above rules. Note that in general nonstandard schemes do not correspond to exact schemes. However, they do offer the opportunity of constructing schemes such that many of the elementary numerical instabilities will not appear. While the above stated rules do not lead to a unique discrete representation of a particular set of differential equations, their application, along with an *a priori* knowledge of significant properties of the solutions to the differential equations, greatly restricts possible discrete models.

APPLICATIONS

In this section, we illustrate both the power and some of the weaknesses of the current stage of constructing nonstandard finite difference schemes.

A Conservative Oscillator

For a single-degree-of-freedom, a general conservative oscillator can be modeled by first writing down its energy function [17]

$$E(x, \dot{x}) = \frac{m\dot{x}^2}{2} + U(x) = \text{constant}, \tag{4.1}$$

and then taking the time derivative to obtain the equation of motion, i.e.

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left(m\ddot{x} + \frac{\mathrm{d}U}{\mathrm{d}x}\right)\dot{x} = 0, \tag{4.2}$$

or

$$m\ddot{x} + \frac{\mathrm{d}U}{\mathrm{d}x} = 0. \tag{4.3}$$

In these expressions m is the mass of the oscillator, $U(x)$ is the potential energy function, $m\dot{x}^2/2$ the kinetic energy and $\dot{x} \equiv \mathrm{d}x/\mathrm{d}t$. Inspection shows that both Eqs. (4.1) and (4.3) are variant under the transformations

$$t \longrightarrow -t \quad \text{(time reversal)}, \tag{4.4a}$$

$$t \longrightarrow t + t_0 \quad \text{(time translation)}. \tag{4.4b}$$

It can be shown that the discrete version of the energy function, $\bar{E}(x_k, x_{k-1})$, should be invariant under the indices interchange [18]

$$k \leftrightarrow k - 1, \tag{4.5}$$

that is

$$\bar{E}(x_k, x_{k-1}) = \bar{E}(x_{k-1}, x_k). \tag{4.6}$$

Thus, given $\bar{E}(x_k, x_{k-1})$, the discrete equation of motion is obtained by applying the Δ operator to the energy equation $\bar{E}(x_k, x_{k-1}) = \text{constant}$, i.e.

$$\Delta\bar{E}(x_k, x_{k-1}) = 0. \tag{4.7}$$

To illustrate this method consider the conservative Duffing equation

$$\ddot{x} + \omega^2 x + \alpha x^2 + \beta x^3 = 0, \tag{4.8}$$

where the energy function is

$$E(x, \dot{x}) = \left(\frac{1}{2}\right)(\dot{x})^2 + \left(\frac{\omega^2}{2}\right)x^2 + \left(\frac{\alpha}{3}\right)x^3 + \left(\frac{\beta}{4}\right)x^4. \tag{4.9}$$

A possible discrete energy function is [18]

$$\bar{E}(x_k, x_{k-1}) = \left(\frac{1}{2}\right)\left[\frac{x_k - x_{k-1}}{\phi(h)}\right]^2 + \left(\frac{\omega^2}{2}\right)x_k x_{k-1} + \left(\frac{\alpha}{3}\right) \times \left(\frac{x_k^2 x_{k-1} + x_k x_{k-1}^2}{2}\right) + \left(\frac{\beta}{4}\right)x_k^2 x_{k-1}^2. \tag{4.10}$$

From $\Delta\bar{E} = 0$, the equation of motion is obtained and is given by

$$\frac{x_{k+1} - 2x_k + x_{k-1}}{[\phi(h)]^2} + \omega^2 x_k + \alpha\left(\frac{x_{k+1} + x_k + x_{k-1}}{3}\right)x_k + \beta x_k^2\left(\frac{x_{k+1} + x_{k-1}}{2}\right) = 0. \tag{4.11}$$

This finite difference scheme has several interesting features:

i) It is linear in x_{k+1} and consequently, the scheme is explicit, i.e. given x_k and x_{k+1}, then x_{k+2} can be determined.
ii) The discrete equation of motion is symmetric in x_{k+1} and x_{k-1}; this is related to the result given in Eqs. (4.5) and (4.6).
iii) Note the very nonlocal discrete representations for the x^2 and x^3 terms, i.e.

$$x^2 \to \left(\frac{x_{k+1} + x_k + x_{k-1}}{3}\right)x_k, \quad x^3 \to x_k^2\left(\frac{x_{k+1} + x_{k-1}}{2}\right). \tag{4.12}$$

The above procedure can be generalized to the case of N-coupled conservative oscillators [19].

Elementary Model for Combustion

The dynamical equation in this case is [20]

$$\frac{du}{dt} = u^2(1 - u), \quad u(0) = u_0 > 0. \tag{4.13}$$

There are three fixed-points

$$\bar{u}^{(1)} = \bar{u}^{(2)} = 0, \quad \bar{u}^{(3)} = 1. \tag{4.14}$$

Referring to Eqs. (3.7) and (3.8), we have

$$R_1 = R_2 = 0, \quad R_3 = 1, \quad R^* = 1, \tag{4.15}$$

and the denominator function

$$\phi(h) = 1 - e^{-h}. \tag{4.16}$$

Thus the discrete derivative is

$$\frac{\mathrm{d}u}{\mathrm{d}t} \to \frac{u_{k+1} - u_k}{1 - \mathrm{e}^{-h}}. \tag{4.17}$$

Now $u(t)$ represents a nonnegative physical quantity, for example, the density of the fuel, and thus the following condition must hold

$$u_k \geq 0 \Rightarrow u_{k+1} \geq 0. \tag{4.18}$$

A way to enforce this requirement is to make the following replacements for u^2 and u^3

$$u^2 \to 2(u_k)^2 - u_{k+1}u_k, \quad u^3 u_{k+1}(u_k)^2. \tag{4.19}$$

Placing these substitutions into Eq. (4.13) gives

$$\frac{u_{k+1} - u_k}{\phi(h)} = 2(u_k)^2 - u_{k+1}u_k - u_{k+1}(u_k)^2, \tag{4.20}$$

which when solved for u_{k+1} is

$$u_{k+1} = \frac{(1 + 2\phi u_k)u_k}{1 + \phi[u_k + (u_k)^2]}. \tag{4.21}$$

Equation (4.13) has the property that all solutions, for $u_0 > 0$, monotonically go to the value $\bar{u}^{(3)} = 1$. This is because the fixed-points $\bar{u}^{(1)}$ and $\bar{u}^{(2)}$ are unstable, while $\bar{u}^{(3)}$ is stable. Using the fact that $\phi(h)$, given by Eq. (4.16) has the property

$$0 < \phi(h) < 1, \quad h > 0, \tag{4.22}$$

it is easy to show that the one dimensional map, Eq. (4.21), has exactly the same properties as the solutions to the combustion equation, i.e.

(1) Equation (4.21) has three fixed-points located at $\bar{u}^{(1)} = \bar{u}^{(2)} = 0$ and $\bar{u}^{(3)} = 1$.
(2) The first two fixed-points are unstable, while the third is stable.

(3) For $u_0 > 0$, the u_k monotonically approach $\bar{u}^{(3)} = 1$. Observe that these three properties hold for all $h > 0$. Thus, the qualitative behavior of the numerical solution has the correct properties independently of the value of the step-size!

HIV Transmission and Control

Nonstandard schemes have been used to numerically integrate a coupled, nonlinear system of ordinary differential equations used to understand the transmission and control of HIV [21,22]. The particular equations to be presented are based on the work of Gumel *et al.* [23].

The model studies four sub-populations, namely: the untreated susceptible population, S_u; the vaccinated susceptible population, S_v; the untreated infected population, Y_u; and the treated (given a drug such as AZT) infected population, Y_v. The total size of the sexually-active population is taken to be

$$N(t) = S_u(t) + S_v(t) + Y_u(t) + Y_v(t). \tag{4.23}$$

The dynamics of this system is given by the following four equations:

$$\frac{dS_u}{dt} = (1 - p\epsilon)\pi - \mu S_u - \frac{c(\beta_1 Y_u + \beta_2 Y_v)S_u}{S_u + S_v + Y_u + Y_v} + \omega S_v, \tag{4.24}$$

$$\frac{dS_v}{dt} = p\epsilon\pi - \mu S_v - \omega S_v - \frac{c(1 - p\epsilon)(\beta_1 Y_u + \beta_2 Y_v)S_v}{S_u + S_v + Y_u + Y_v}, \tag{4.25}$$

$$\frac{dY_u}{dt} = \frac{c(\beta_1 Y_u + \beta_2 Y_v)S_u}{S_u + S_v + Y_u + Y_v} - \mu Y_u - d_1 Y_u - \tau Y_u, \tag{4.26}$$

$$\frac{dY_v}{dt} = \frac{c(\beta_1 Y_u + \beta_2 Y_v)S_v}{S_u + S_v + Y_u + Y_v} - \mu Y_v - d_2 Y_v + \tau Y_u. \tag{4.27}$$

Our nonstandard scheme for Eqs. (4.24)–(4.27) is

$$\frac{S_u^{k+1} - S_u^k}{h} = (1 - p\epsilon)\pi - \mu S_u^{k+1} - \frac{c(\beta_1 Y_u^k + \beta_2 Y_v^k)S_u^{k+1}}{S_u^k + S_v^k + Y_u^k + Y_v^k} + \omega S_v^k, \tag{4.28}$$

$$\frac{S_v^{k+1} - S_v^k}{h} = p\epsilon\pi - \mu S_v^{k+1} - \omega S_v^{k+1} - \frac{c(1 - p\epsilon)(\beta_1 Y_u^k + \beta_2 Y_v^k)S_v^{k+1}}{S_u^{k+1} + S_v^k + Y_u^k + Y_v^k}, \tag{4.29}$$

$$\frac{Y_u^{k+1} - Y_u^k}{h} = \frac{c\left[\beta_1(2Y_u^k - Y_u^{k+1}) + \beta_2 Y_v^k\right]S_u^{k+1}}{S_u^{k+1} + S_v^{k+1} + Y_u^k + Y_v^k} - \mu Y_u^{k+1} - d_1 Y_u^{k+1} - \tau Y_u^{k+1}, \tag{4.30}$$

$$\frac{Y_v^{k+1} - Y_v^k}{h} = \frac{c\beta_1 Y_u^{k+1} S_v^{k+1} + c\beta_2(2Y_v^k - Y_v^{k+1})S_v^{k+1}}{S_u^{k+1} + S_v^{k+1} + Y_u^{k+1} + Y_v^k} - \mu Y_v^{k+1} - d_2 Y_v^{k+1} + \tau Y_u^{k+1}. \tag{4.31}$$

The parameters (β_1, β_2, c, d_1, d_2, p, μ, ϵ, π, τ, ω) are all positive. These equations can be, respectively, solved for the dependent variable at the discrete-time t_{k+1}. Carrying out this calculation gives four equations of the form

$$S_u^{k+1} = F(S_u^k, S_v^k, Y_u^k, Y_v^k), \tag{4.32}$$

$$S_v^{k+1} = G(S_u^{k+1}, S_v^k, Y_u^k, Y_v^k), \tag{4.33}$$

$$Y_u^{k+1} = H(S_u^{k+1}, S_v^{k+1}, Y_u^k, Y_v^k), \tag{4.34}$$

$$Y_v^{k+1} = I(S_u^{k+1}, S_v^{k+1}, Y_u^{k+1}, Y_v^k). \tag{4.35}$$

The structure of these equations are such that if the values for $(S_u^k, S_v^k, Y_u^k, Y_v^k)$ are nonnegative, then their values are nonnegative at t_{k+1}.

To obtain numerical solutions, S_u^{k+1} is calculated from $(S_u^k, S_v^k, Y_u^k, Y_v^k)$; S_v^{k+1} is next determined by using this value for S_u^{k+1} and those of (S_v^k, Y_u^k, Y_v^k) in Eq. (4.33). Subsequent calculations repeat this process for Y_u^{k+1} and Y_v^{k+1}. In summary, given $(S_u^k, S_v^k, Y_u^k, Y_v^k)$, the calculation of the dependent variables at the t_{k+1}, discrete-time, proceeds in the order

$$S_u^{k+1} \to S_v^{k+1} \to Y_u^{k+1} \to Y_v^{k+1}. \tag{4.36}$$

Extensive numerical simulations were carried out using realistic estimates for the various parameters. For purposes of comparison, the RK4 method was used to also solve the initial value problem, i.e. the S_u^0, S_v^0, Y_u^0, and Y_v^0 are given. In all of the tests, the above derived nonstandard scheme outperformed the standard RK4 method.

It should be noted that our nonstandard scheme used a simple forward-Euler approximation for the first-order time derivatives. For this system the use of a more complex denominator function was not required. The

standard selection, $\phi(h) = h$, worked quite well. As a check, the numerical simulations were run with h in the range, $0.001 \leq h \leq 10^6$, and in each case the nonstandard scheme always gave solutions that converged to the correct fixed-point.

Fisher Equation

Another of the famous partial differential equations used to test numerical integration methods is the Fisher equation

$$u_t = u_{xx} + u(1 - u). \tag{4.37}$$

The physically relevant solutions are those that satisfy the condition

$$0 \leq u(x, 0) \leq 1 \Rightarrow 0 \leq u(x, t) \leq 1, \quad t > 0. \tag{4.38}$$

We would like to have the nonstandard scheme also satisfy this requirement.

A possible nonstandard finite difference scheme for the Fisher equation is

$$\frac{u_m^{k+1} - u_m^k}{\Delta t} = \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{(\Delta x)^2} + 2\bar{u}_m^k - u_m^{k+1} - \bar{u}_m^k u_m^{k+1}, \tag{4.39}$$

where the simplest choice was made for the two denominator functions, i.e.

$$\phi_1(\Delta t) = \Delta t, \quad \phi_2(\Delta x) = (\Delta x)^2, \tag{4.40}$$

and the variable $\bar{u}_m^k$ is defined to be

$$\bar{u}_m^k \equiv \frac{u_{m+1}^k + u_m^k + u_{m-1}^k}{3}. \tag{4.41}$$

Note that the following discrete, nonlocal representations were used for the u and u^2 terms,

$$u = 2u - u \rightarrow 2\bar{u}_m^k - u_m^k, \quad u^2 \rightarrow \bar{u}_m^k u_m^{k+1}. \tag{4.42}$$

Since u_m^{k+1} appears linearly in Eq. (4.39), it can be solved for to obtain the explicit scheme, for $R = \Delta t/(\Delta x)^2 = 0.5$,

$$u_m^{k+1} = \frac{(0.5)(u_{m+1}^k + u_{m-1}^k) + (2\Delta t)\bar{u}_m^k}{1 + \Delta t + (\Delta t)\bar{u}_m^k}. \tag{4.43}$$

In general, only the restriction $R \leq 0.5$ is required to enforce the positivity condition.

An important feature of this scheme is that its solutions also satisfy a boundedness condition; see Eq. (4.38). The proof of this result is very direct. First, require u_m^k to have the property $0 \leq u_m^k \leq 1$. From this it follows that

$$\left(\frac{1}{2}\right)(u_{m+1}^k + u_{m-1}^k) \leq 1, \tag{4.44}$$

and

$$(2\Delta t)\bar{u}_m^k = (\Delta t)\bar{u}_m^k + (\Delta t)\bar{u}_m^k \leq \Delta t + (\Delta t)\bar{u}_m^k. \tag{4.45}$$

Adding Eqs. (4.44) and (4.45) gives

$$\left(\frac{1}{2}\right)(u_{m+1}^k + u_{m-1}^k) + (2\Delta t)\bar{u}_m^k \leq 1 + \Delta t + (\Delta t)\bar{u}_m^k. \tag{4.46}$$

Dividing the inequality by $1 + \Delta t + (\Delta t)\bar{u}_m^k$, gives

$$\frac{\left(\frac{1}{2}\right)(u_{m+1}^k + u_{m-1}^k) + (2\Delta t)\bar{u}_m^k}{1 + \Delta t + (\Delta \mathrm{t})\bar{u}_m^k} \leq 1. \tag{4.47}$$

However, the left-side of the expression in Eq. (4.47) is u_m^{k+1}. Consequently, it follows (by induction) that

$$0 \leq u_m^0 \leq 1 \Rightarrow 0 \leq u_m^k \leq 1, \quad k \geq 1, \tag{4.48}$$

and all relevant values of m.

The following nonlinear equation has been used study propagation problems related to laminar flow in combustion [25]

$$u_t = u_{xx} + u^2(1 - u). \tag{4.49}$$

This equation is a modified Fisher equation and the techniques used for that equation can be applied to it. A possible nonstandard scheme is obtained by making the following replacements [9]

$$u^2 = 2u^2 - u^2 \rightarrow \left(u_{m+1}^k\right)^2 + \left(u_{m-1}^k\right)^2 - \left(\frac{u_{m+1}^k + u_{m-1}^k}{2}\right)u_m^{k+1}, \tag{4.50a}$$

$$u^3 \rightarrow \left[\frac{(u_{m+1}^k)^2 + (u_{m-1}^k)^2}{2}\right]u_m^{k+1}, \tag{4.50b}$$

$$u_t \to \frac{u_m^{k+1} - u_m^k}{\Delta t}, \quad u_{xx} \to \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{(\Delta x)^2}. \tag{4.50c}$$

Making these substitutions into Eq. (4.49) and solving for u_m^{k+1} gives

$$u_m^{k+1} = \frac{R\left(u_{m+1}^k + u_{m-1}^k\right) + (\Delta t)\left[(u_{m+1}^k)^2 + (u_{m-1}^k)^2\right] + (1 - 2R)u_m^k}{1 + \left(\frac{\Delta t}{2}\right)\left[u_{m+1}^k + (u_{m+1}^k)^2 + u_{m-1}^k + (u_{m-1}^k)^2\right]} \tag{4.51}$$

where $R = \Delta t/(\Delta x)^2$. Examination of Eq. (4.51) shows that if u_m^k is nonnegative, then u_m^{k+1} will also be nonnegative provided

$$1 - 2R \geq 0. \tag{4.52}$$

Selecting the equal sign, the following relation holds between the step-sizes

$$\Delta t = \frac{(\Delta x)^2}{2}, \tag{4.53}$$

and Eq. (4.51) becomes

$$u_m^{k+1} = \frac{(0.5)\left(u_{m+1}^k + u_{m-1}^k\right) + (\Delta t)\left[(u_{m+1}^k)^2 + (u_{m-1}^k)^2\right]}{1 + \left(\frac{\Delta t}{2}\right)\left[u_{m+1}^k + (u_{m+1}^k)^2 + u_{m-1}^k + (u_{m-1}^k)^2\right]}. \tag{4.54}$$

It can be demonstrated that [9]

$$0 \leq u_m^k \leq 1 \Rightarrow 0 \leq u_m^{k+1} \leq 1, \tag{4.55}$$

for fixed k and over all values of m. Consequently, the above nonstandard scheme satisfies both the positivity and boundedness conditions.

Simple Isothermal Chemical System

In dimensionless form the dynamics of a simple isothermal chemical system can be modeled by the following pair of nonlinear partial differential equations [26]

$$u_t = u_{xx} - uw, \tag{4.56}$$

$$w_t = w_{xx} + uw - hw, \tag{4.57}$$

where h is a positive parameter. Twizell *et al.* [26] made a detailed study of various explicit and implicit finite difference schemes for these equations. They concluded that finite difference schemes can produce chaotic

behavior in the numerical solutions, in spite of the fact that these differential equations are not expected to have such behaviors for their solutions. We have constructed nonstandard schemes and find no chaotic solutions. The scheme used for numerical experiments is given by the following expressions

$$\frac{u_m^{k+1} - u_m^k}{\Delta t} = \frac{u_{m+1}^k - 2u_m^k + u_{m-1}^k}{(\Delta x)^2} - u_m^{k+1} u_m^k, \tag{4.58}$$

$$\frac{w_m^{k+1} - w_m^k}{\Delta t} = \frac{w_{m+1}^k - 2w_m^k + w_{m-1}^k}{(\Delta x)^2} + 2u_m^k w_m^k - u_m^k w_m^{k+1} - h w_m^{k+1}. \tag{4.59}$$

Solving for u_m^{k+1} and w_m^{k+1} gives

$$u_m^{k+1} = \frac{R(u_{m+1}^k + u_{m-1}^k) + (1 - 2R)u_m^k}{1 + (\Delta t)w_m^k}, \tag{4.60}$$

$$w_m^{k+1} = \frac{R(w_{m+1}^k + w_{m-1}^k) + (2\Delta t)u_m^k w_m^k + (1 - 2R)w_m^k}{1 + (\Delta t)(h + u_m^k)}. \tag{4.61}$$

Note that the positivity requirement is satisfied if

$$1 - 2R \geq 0 \Rightarrow \Delta t \leq \frac{(\Delta x)^2}{2}. \tag{4.62}$$

In our numerical experiments, we used $R = 0.5$ [27].

An alternative expression can be obtained by replacing u_m^k with u_m^{k+1} in Eqs. (4.59) and (4.61). In this case, u_m^{k+1} is calculated first and then used to determine w_m^{k+1}.

Unplugged Van Der Pol Equation

The van der Pol equation with no energy input, i.e. "unplugged", takes the form [28]

$$\ddot{x} + x = -\mu x^2 \dot{x}, \tag{4.63}$$

where $\dot{x} = \mathrm{d}x/\mathrm{d}t$, etc.; and μ is a positive parameter. Using an energy argument, it can be shown that all solutions to Eq. (4.63) oscillate with an amplitude that monotonically goes to zero.

The application of elementary methods of numerical integration to Eq. (4.63) do not give results that are consistent with the known properties of its solutions. In fact, the forward Euler method produces a scheme for which the fixed point in the $(x, y = \dot{x})$ phase space is always unstable [29]. Thus, for this method, the dynamics of the discrete equations are clearly inconsistent with those of the original equation (4.63). However, the direct application of nonstandard techniques leads to a scheme that is dynamically consistent with the differential equation.

To proceed, rewrite Eq. (4.63) in the following system form

$$\frac{\mathrm{d}x}{\mathrm{d}t} = y - \left(\frac{\mu}{3}\right)x^3, \quad \frac{\mathrm{d}y}{\mathrm{d}t} = -x. \tag{4.64}$$

The scheme selected for Eq.(4.64) is

$$\frac{x_{k+1} - x_k}{\phi} = y_k - \left(\frac{\mu}{3}\right)x_k^3, \quad \frac{y_{k+1} - y_k}{\phi} = -x_{k+1}, \tag{4.65}$$

with

$$\phi = 2\sin\left(\frac{h}{2}\right), \quad h = \Delta t. \tag{4.66}$$

Eliminating the y_k variable gives a second-order equation for x_k, i.e.

$$\frac{x_{k+1} - 2x_k + x_{k-1}}{\phi^2} + x_k = -\mu\left(\frac{x_k^2 + x_k x_{k-1} + x_{k-1}^2}{3}\right)\left(\frac{x_k - x_{k-1}}{\phi}\right). \tag{4.67}$$

Note that the x^2 expression in Eq. (4.64) was replaced by

$$x^2 \rightarrow \frac{x_k^2 + x_k x_{k-1} + x_{k-1}^2}{3}, \tag{4.68}$$

and that the first-order time derivative is modeled by a backward-Euler representation. Our numerical experiments showed that the nonstandard scheme of Eq. (4.65) gave solutions with the correct dynamical behavior. Also, we were able to obtain a restriction on the maximum step-size, h^*, that could be used. For the initial conditions

$$x(0) = x_0, \quad \dot{x}(0) = -y(0) = 0, \tag{4.69}$$

this was

$$h^* = \frac{6}{\mu x_0^2}. \tag{4.70}$$

DISCUSSION

Nonstandard finite difference schemes are beginning to have an impact on the field of the numerical integration of differential equations. In particular, such schemes have been constructed and applied to the wave and Maxwell's equations [30], subsurface biobarrier formation in porous media [31,32], and convective–dispersive transport problems with nonlinear reaction [33]. Further, initial work has begun on placing the mathematical foundation of the subject on a firm basis [34,35]. To date our investigations have centered on constructing nonstandard schemes that incorporate the important dynamical properties of the original differential equations such as positivity and/or conservation requirements. We have not attempted to find, in some sense, the best or optimal discrete models for the differential equations. However, there does exist strong hints as to how to proceed with this task [36].

In conclusion, we list several problems for which further work is needed:

(1) A very difficult problem is the construction of a proper nonstandard scheme for systems of ordinary differential equations when a fixed-point exists with neutral stability.

(2) Partial differential equations having nonlinear advection and/or diffusion terms occur in the mathematical modeling of many systems in the chemical, biological, and engineering sciences [24]. Very little work has been done on constructing nonstandard schemes for such equations. In particular, it would be of interest to determine if schemes can always be constructed such that they are "explicit" in the dependent variables. We have already demonstrated that this is the case if a linear advection term is present [37]. For one-space dimension, the general scalar equation takes the form

$$u_t + [f(u)]_x = [D(u)u_x]_x + g(u), \tag{5.1}$$

where $g(u)$ is the reaction term, $D(u)$ is a dependent variable diffusion function, and $f(u)$ is a nonlinear function of u.

(3) Finally, all of these procedures, obtained and studied for one-space dimension need to be generalized to higher dimensional systems. Preliminary work suggests that while this is possible, the algebraic and other calculational details increase rapidly with the space-dimension number [38].

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