CHAPTER 1

NONSTANDARD FINITE DIFFERENCE METHODS

Ronald E. Mickens
Clark Atlanta University
Box 172 – Physics Department
Atlanta, GA 30314, USA
rohrs@math.gatech.edu

A brief history of nonstandard finite difference (NSFD) methods is given along with clarifying remarks related to the views of some others on these techniques. We also present the basic rules governing the formulation of NSFD schemes and discuss the concept of dynamic consistency and its role in the construction of such schemes. A list of some outstanding problems is given to indicate possible future research directions for the continued investigation of NSFD for the purpose of numerical integration of differential equations.

1. General Comments

Nonstandard finite difference (NSFD) methods for the numerical integration of differential equations had their genesis in a paper published in 1989 [1]. The basic rules to construct such schemes [2] and their application to specific nonlinear equations appear in a variety of publications [3,4]. In recent years, NSFD discrete models have been constructed and/or tested for a wide range of nonlinear dynamical systems:

- singular boundary value problems expressed in cylindrical or spherical coordinates [5],
- a generalized Nagumo reaction-diffusion model [6],
- equations modeling stellar structure [7],
- the dynamics of HIV transmission [8],
- modified linear heat/diffusion transport problems [9].

ADVANCES IN THE APPLICATIONS OF NONSTANDARD FINITE DIFFERENCE SCHEMES

An essentially complete listing and summary of publications using NSFD methods, up to 2004, is presented in the paper by Patidar [10]. This paper [10] and other published works [3]–[9] provide ample evidence that NSFD schemes are enjoying a growing applicability as the practical users of numerical techniques for differential equations become aware of the advantages and power of these methods. However, there is the view, held by some individuals [11,12], that the NSFD method depends on "using the known solution of the differential equation or by '*ad hoc*' experimentation . . . " [12]. A detailed study and examination of the results produced to date easily show this interpretation of what has been accomplished using NSFD methods to be false.

An essential issue, coming from both my work and of others on NSFD methods, is the realization that each differential equation has to be considered a "unique" mathematical structure and, consequently, must be discretely modeled in a unique manner. This is a very important aspect of NSFD methods and the contributors to this book illustrate this point in their presented works.

In the next section, we give a brief outline of the basic rules defining the fundamental techniques that generate NSFD schemes for differential equations. This is followed, in Section 3, by a similar brief discussion of the principle of dynamic consistency. Since excellent and extensive published presentations already exist on these two topics [2,3,13,14], there is no need to provide full information here on this topic.

2. NSFD Methods: Basic Principles

Detailed studies of so-called exact finite difference schemes [2] form the foundation of NSFD methods [1,2,15]. The extension and generalization of these results to special groups of differential equations for which exact schemes are not available has also provided additional insight into the required structural properties of NSFD methods [16]. Based on this work, the following rules for constructing nonstandard schemes follow:

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

Comment 1. If the orders of the discrete derivatives are larger than those occurring in the differential equations, then numerical instabilities will in general occur [2,17].

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

Comment 2. Consider the first-order derivative of $x(t)$ and its discrete analog; its most general form is

$$\frac{dx}{dt} \to \frac{x_{k+1} - \psi(h)x_k}{\phi(h)}\,, \tag{1}$$

where ψ and ϕ are functions of the step-size, $h = \Delta t$, and are called, respectively, the "numerator" and "denominator" functions; $t_k = hk$, and $x(t) \to x_k$; and where the (ψ, ϕ) have the properties

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

Note that conventional discrete representation for the first derivative take $\psi(h) = 1$ and $\phi(h) = h$ [17]. For systems of coupled, first-order, ordinary differential equations there exists a systematic method for constructing denominator functions [2,16]. Also, unless the "system" has dissipation, the numerator function is usually equal to one [2].

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

Comment 3. The simplest illustration of this requirement is the logistic equation, i.e.,

$$\frac{dx}{dt} = x(1 - x). \tag{3}$$

A straightforward standard discretization gives

$$\frac{x_{k+1} - x_k}{h} = x_k(1 - x_k). \tag{4}$$

This equation can be transformed into the logistic difference equation [2]

$$z_{k+1} = \lambda z_k(1 - z_k), \qquad \lambda = 1 + h \tag{5}$$

which has periodic and chaotic solutions, and thus cannot be a valid discrete model for Eq. (3). However, the use of a nonlocal representation for x^2, i.e.,

$$x^2 \to x_{k+1}x_k\,, \tag{6}$$

gives

$$\frac{x_{k+1} - x_k}{h} = x_k(1 - x_{k+1}), \tag{7}$$

or

$$x_{k+1} = \left(\frac{1 + h}{1 + hx_k}\right) x_k. \tag{8}$$

This discrete model gives numerical solutions for Eq. (3) that are qualitatively correct for $x_0 > 0$ and all $h > 0$; see Mickens [2].

Rule 4. Special conditions that hold for either the differential equation and/or its solutions should also hold for the difference equation model and/or its solutions.

Comment 4. An example is an ordinary differential equation for which the substitution, $t \to -t$, leaves the equation invariant. If the discrete model does not also have this property, then numerical instabilities may occur.

Comment 5. In general, numerical instabilities are solutions to the discrete equations that do not correspond to any solution of the corresponding differential equations.

Definition. A nonstandard finite difference scheme is any discrete representation of a system of differential equations that is constructed based on the above rules.

3. Dynamic Consistency

Dynamic consistency (DC) is an important concept that can be used to guide the construction of valid discrete models for differential equations. DC is always formulated in terms of particular properties of a system [13,18]. Below, we define DC in terms of ordinary differential equations (DOE); however, it should be clear that the definition can be easily extended to partial differential equations (PDE).

Definition

Consider the differential equation

$$\frac{dx}{dt} = f(x, t, \lambda), \tag{9}$$

where λ represents the parameters defining the system modeled by Eq. (9). Let a finite difference scheme for Eq. (9) be

$$x_{k+1} = F(x_k, t_k, h, \lambda). \tag{10}$$

Let the differential equation and/or its solutions have property P. The discrete model, Eq. (10), is dynamically consistent with Eq. (9), if it and/or its solutions also has property P.

Comment 6. For many systems in the natural and engineering sciences, properties of particular importance include [19,20,21]:

- positivity
- boundedness
- monotonicity
- fixed-points and their stability properties
- integer valued dependent variables

- existence of special solutions (traveling waves, solitons, rational, etc.)
- limit cycles and other periodic solutions.

A given system might include one or more of these properties or others not listed. The critical issue is that a valid finite difference model will not exist unless all of the essential properties of the original differential equations are incorporated into it. From this viewpoint, it follows that the existence of numerical instabilities is an indication that some "physical principle" underlying the dynamics of the original system is not included in the discrete model.

Comment 7. Let, for the same initial conditions, $x(t)$ and x_k be the solutions, respectively, to Eqs. (9) and (10). If for any time step-size, $h > 0$, we have

$$x(t_k) = x_k, \tag{11}$$

then Eq. (10) is an exact difference scheme for Eq. (9) [2].

Comment 8. Note that NSFD rule 4, given in the previous section, incorporates the principle of DC.

To illustrate the use of DC in the construction of NSFD schemes, consider the decay equation

$$\frac{dx}{dt} = -\lambda x, \qquad x(0) = x_0, \tag{12}$$

where λ is a positive parameter. Applying the qualitative theory of differential equations [22], it can be directly shown, even without knowledge of the explicit solution, that solutions to Eq. (12) have the following properties:

P_1 − $x(t) = 0$ is a fixed-point;

P_2 − given $x_0 \neq 0$, then $x_0 x(t) > 0$ for $t > 0$;

P_3 − $x(t)$ monotonically decreases in magnitude to zero for any $x_0 \neq 0$.

The standard forward-Euler scheme

$$\frac{x_{k+1} - x_k}{h} = -\lambda x_k \quad \text{or} \quad x_{k+1} = (1 - \lambda h)x_k, \tag{13}$$

violates P_2 and P_3 if λh is sufficiently large. Consequently, this scheme is not DC with Eq. (12). However, the NSFD scheme

$$\frac{x_{k+1} - x_k}{\phi(h)} = -\lambda x_k, \qquad \phi(h) = \frac{1 - e^{-\lambda h}}{\lambda}, \tag{14}$$

can be easily demonstrated to satisfy P_1, P_2, and P_3 for all step-sizes, $h > 0$. (This scheme follows directly from the work given in Mickens [16]; see also

Mickens [2].) Thus, the NSFD scheme of Eq. (14) is DC with Eq. (12). Another interesting feature of this representation is that it is also an exact finite difference scheme for Eq. (12); see Mickens [2].

The publications [6,7,8,9,13,14,18] provide a wide range of the application of the principle of DC to differential equations for which the property of positivity holds.

4. Some Outstanding Problems

Progress in the creation/construction/understanding of the NSFD set of procedures requires the investigation of a set of related issues. The following is a listing of some of the problems for which resolution is needed.

1) Coupled ODE's having fixed-points that are either linear or nonlinear centers are very difficult to deal with in an efficient manner [23,24,25]. Such systems may have several time scales. Also the numerical computed periods of oscillations can depend on the time step-size [24]. One consequence is that the integration step-size must be small relative to these scales if the computed numerical solutions are to give meaningful solutions. Violation of this restriction will always give "physically meaningless" solutions.

2) To date, essentially all of the NSFD schemes have been studied for one-space dimension systems. Thus, it is of great importance to see how the current techniques can be extended to higher space dimension equations. Preliminary results show that the algebraic work increase rapidly with an increase in the number of space variables [26,27].

3) To date, little effort has gone into the investigation of implicit schemes, especially for PDE's [2]. One way to proceed would be to reconsider some of the model linear and nonlinear PDE's already studied using explicit methods. A restriction to be placed on these implicit schemes is to have all the variables, evaluated at the advanced discrete-time level, appear linearly in the discrete finite difference equations.

4) Cross-diffusion occurs when, in a system of coupled PDE's the diffusion coefficients depend on variables other than those appearing in the evolutionary term of a particular equation. Such terms regularly occur in the dynamics of cancer [28] and the spatial interactions of several populations [29,30]. An example of such a set of equations is [28]

$$\frac{\partial u}{\partial t} = u(1-u) - \frac{\partial}{\partial x}\left(u\,\frac{\partial c}{\partial x}\right), \qquad \frac{\partial c}{\partial t} = -uc^2, \tag{15}$$

where $u(x,t)$ and $c(x,t)$ satisfy a positivity condition, i.e.,

$$u(x,0) \geq 0, \quad c(x,0) \geq 0 \Rightarrow u(x,t) \geq 0, \quad c(x,t) \geq 0 \qquad \text{for } t > 0. \tag{16}$$

The second term on the right-side of the "u"-evolution equation is the cross-diffusion term. The issue to be studied is how to construct NSFD schemes such that the positivity condition, Eq. (16), holds for the solutions to the discrete equations.

5) The NSFD schemes to date have been of rather low order accuracy in the step-sizes. Procedures exist to calculate second-order accurate NSFD models [27]. However, such efforts so far give schemes that may violate the positivity condition. This is a fundamental problem whose solution is still unknown.

6) Finally, it should be mentioned that a firm theoretical basis is needed to fully understand NSFD methods. Some progress in this direction is being made by Jean M.-S. Lubuma and his collaborators [31].

Acknowledgements

The results given in this chapter have been supported over the previous several decades by research grants from ARO, DOE, NASA, and NIH-MBRS. I wish to thank a number of collaborators for their stimulating scientific discussions and research productivity in the area of NSFD methods: Abba B. Gumel (University of Manitoba), Pedro M. Jordan (NRL, Stennis Space Center), Kale Oyedeji (Morehouse College), and Sandra A. Rucker (Clark Atlanta University). I also would like to acknowledge several individuals who through their work has influenced and helped shape my own current views of NSFD methods and related issues: Ron Buckmire (Occidental College) and Jean M.-S. Lubuma (University of Pretoria).

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