Mathl Comput. Modelling, Vol. 11, pp. 528–530, 1988
Printed in Great Britain

0895-7177/88 $3.00 + 0.00
Pergamon Press plc

LIE METHODS IN MATHEMATICAL MODELLING

DIFFERENCE EQUATION MODELS OF DIFFERENTIAL EQUATIONS

Ronald E. Mickens

Departments of Physics and Mathematics
Atlanta University, Atlanta, Georgia 30314

Abstract. For purposes of numerical integration, differential equations are often modeled by finite-differences. However, these models raise a number of questions related to how the finite-difference schemes are to be constructed, the magnitude of the local truncation errors, the existence and elimination of numerical instabilities, etc. We prove a theorem which states that to each ordinary differential equation there corresponds an "exact" finite-difference scheme, i.e., the local truncation error is zero. This means that on the computational grid or lattice, the solution to the difference equation is exactly equal to the solution to the differential equation. We use the theorem to show, by means of a number of explicit examples, that the usual rules for constructing finite-difference schemes are "wrong." Several modeling principles are presented, as well as their application to partial differential equations.

Keywords. Difference equations; differential equations; numerical analysis; mathematical modeling.

INTRODUCTION

Differential equations arise in the mathematical modeling and analysis of dynamic systems (Drazin, 1983; Potter, 1973). The usual situation is that seldom are general exact analytical solutions known. Thus, interest may center on special solutions, i.e., singular or equilibrium solutions, traveling wave solutions, etc. Often approximations to exact solutions can be determined using perturbation procedures and related expansion techniques (Mickens, 1981; Nayfeh, 1973; Jordan and Smith, 1977). Numerical integration of the differential equations can also be done using a variety of procedures; one of particular importance is the use of finite-differences to model the relevant differential equations (Potter, 1973; Richtmyer and Morton, 1967). However, finite-difference techniques have inherent within them a number of potential problems.

First, the whole modeling procedure is non-unique. For example, the derivative dx(t)/dt can be replaced by any one of the following expressions (Potter, 1973)

$$\frac{x_{k+1}-x_k}{h} + O(h), \quad \frac{x_{k+1}-x_{k-1}}{2h} + O(h^2), \qquad (1)$$

where $h = \Delta t$ is the step-size and $x_k = x(hk)$. Note that the derivative is always modeled non-locally, i.e., its finite-difference equivalence is "spread" over two or more grid points. However, nonlinear terms, such as x^2, can be represented either locally, i.e., as x_k^2, or nonlocally, e.g., as $x_{k+1}x_k$ (Mickens, 1984).

Second, the inappropriate modeling of a differential equation (DE) by a difference equation (ΔE) can lead to both "ghost solutions" (Ushiki, 1982) and numerical instabilities (Richtmyer and Morton, 1967). In fact, careless procedures can produce ΔE models of DE's such that chaotic behavior appears for all step-sizes (Ushiki, 1982). All of these problems are related to the issues of convergence, stability and consistency which arise in the use and analysis of finite-difference schemes (Richtmyer and Morton, 1967).

In the following, we prove that every ordinary DE has a corresponding "exact" ΔE model such that on the computational grid or lattice the solution to the ΔE is exactly equal to the solution to the DE. Further, this holds independently of the step-size. We then use this result to show, by means of a number of explicit examples, that the usual rules for constructing ΔE models of DE's are "wrong." We conclude with the listing of several modeling principles. The results presented here are an extension of previous work by the author (Mickens, 1984).

EXACT DIFFERENCE SCHEMES

Consider a first-order ordinary differential equation (ODE)

$$\frac{dx}{dt} = f(t,x), \quad x_0 = x(t_0), \qquad (2)$$

and a first-order ordinary difference equation (OΔE)

$$x_{k+1} = g(k,x_k). \qquad (3)$$

Let $t_k = hk$, for $h > 0$. Equations (2) and (3) are said to have the same general solution if and only if

$$x_k = x(hk), \qquad (4)$$

for arbitrary constant values of h (Potts, 1982a; Mickens, 1984). An exact difference scheme is one for which the solution to the OΔE has the same general solution as the associated ODE.

We now prove an interesting theorem: Every ODE has an exact difference scheme. The proof consists of the actual construction of such a difference scheme. Let f(x,t), in Eq. (2) have the necessary properties such that a solution, $x(t) = \phi(x_0,t_0,t)$, exists. Now, the "group property" (Nemytski and Stepanov, 1969) of the solutions to Eq. (2) gives

$$x(t+h) = \phi[x(t),t,t+h], \tag{5}$$

where h is an arbitrary constant. If we now make the identifications

$$t \to t_k = hk, \quad x(t) \to x_k = x(hk), \tag{6}$$

then Eq. (5) becomes

$$x_{k+1} = \phi[x_k,hk,h(k+1)]. \tag{7}$$

This is the required OΔE which has the same general solution as Eq. (2).

Note that we have only obtained an existence theorem, i.e., exact finite-difference schemes exists for ODE's. Consequently, in practice, the theorem itself cannot be used to directly construct an exact difference scheme for a given ODE. However, we can apply this theorem to differential equations with known solutions and use these results to study the various possible modeling behaviors of derivatives and nonlinear terms. From this exercise, we can obtain useful information on modeling rules for realistic situations where exact solutions are not known a priori.

EXAMPLES

Using the results of the previous section, we now consturct exact difference schemes for a number of ODE's. While we do not give the actual details of the construction for each equation, it should be obvious from Eq. (7) how this is done. In summary: (i) The general solution to the initial value problem for the ODE is obtained, i.e., $x(t) = \phi(x_0,t_0,t)$. (ii) The substitutions, $x(t) \to x_{k+1}$, $t_0 \to hk$, $t \to h(k+1)$, then gives the desired OΔE.

In the following, we list the ODE and its best difference scheme; λ,ω, etc. are constants and P(t) is an integrable function of t.

$$\frac{dx}{dt} = -\lambda x, \tag{8a}$$

$$\frac{x_{k+1} - x_k}{\left(\frac{1-eh^{-\lambda h}}{\lambda}\right)} = -\lambda x_k; \tag{8b}$$

$$\frac{dx}{dt} = P(t)x, \tag{9a}$$

$$\frac{x_{k+1}-x_k}{h} = \left[\exp \int_{hk}^{h(k+1)} P(z)dz - 1\right]x_k/h; \tag{9b}$$

$$\frac{dx}{dt} = P(t)x^2, \tag{10a}$$

$$\frac{x_{k+1}-x_k}{h} = \left[\int_{hk}^{h(k+1)} P(z)dz/h\right]x_k x_{k+1}; \tag{10b}$$

$$\frac{dx}{dt} = x(1-x); \tag{11a}$$

$$\frac{x_{k+1}-x_k}{(1-e^{-h})} = x_{k+1}(1-x_k); \tag{11b}$$

$$\frac{dx}{dt} = -\sqrt{x}, \tag{12a}$$

$$\frac{x_{k+1}-x_k}{h} = \left[\frac{\sqrt{x_{k+1}} + \sqrt{x_k}}{2}\right]; \tag{12b}$$

$$\frac{dx}{dt} = -\lambda x \mathrm{LN}\left(\frac{x}{m}\right), \tag{13a}$$

$$\frac{x_{k+1}-x_k}{h} = -\lambda x\left[\frac{1-\left(\frac{x_k}{m}\right)^{(e^{-\lambda h}-1)}}{h}\right]; \tag{13b}$$

$$2\frac{dx}{dt} + x = \frac{1}{x}, \tag{14a}$$

$$2\left[\frac{x_{k+1}-x_k}{1-e^{-h}}\right] + \frac{x_k^2}{\left(\frac{x_{k+1}+x_k}{2}\right)} = \frac{1}{\left(\frac{x_{k+1}+x_k}{2}\right)}; \tag{14b}$$

$$\frac{d^2x}{dt^2} = \lambda \frac{dx}{dt}, \tag{15a}$$

$$\frac{x_{k+1}-2x_k+x_{k-1}}{\left(\frac{e^{\lambda h}-1}{\lambda}\right)h} = \lambda\left[\frac{x_k-x_{k-1}}{h}\right]; \tag{15b}$$

$$\frac{d^2x}{dt^2} + \omega^2 x = 0, \tag{16a}$$

$$\frac{x_{k+1}-2x_k+x_{k-1}}{\left(\frac{4}{\omega^2}\right)\sin^2\left(\frac{\omega h}{2}\right)} + \omega^2 x_k = 0; \tag{16b}$$

$$\frac{dx}{dt} = -x^3, \tag{17a}$$

$$\frac{x_{k+1}-x_k}{h} = -\left[\frac{2x_{k+1}}{x_{k+1}+x_k}\right]x_{k+1}x_k^2; \tag{17b}$$

$$\frac{dx}{dt} = \tan x, \tag{18a}$$

$$\frac{x_{k+1}-x_k}{h} = \frac{\sin^{-1}[e^h \sin x_k] - x_k}{h}. \tag{18b}$$

MODELING RULES

Given an ODE, how should we proceed to construct a finite-difference model? The following rules/ideas are based on both analytic and numerical studies of a large number of linear and nonlinear ODE's. The reader can refer to the results of the last section to verify directly certain of these procedures.

Rule 1. The order of the ΔE must be equal to the order of the DE. Violation of this rule means that "ghost solutions" will appear (Ushiki, 1982).

Rule 2. Nonlinear (power) terms should be modeled nonlocally on the computational grid. See Eqs. (10), (11) and (17) and Potts (1982b, 1987).

Rule 3. Denominator functions in the modeling of derivatives must, in general, be expressed in terms of more complicated functions of the step-size than those conventionally used (Richtmyer and Morton, 1967). See Eqs. (8), (11), (14), (15) and (16).

Rule 4a. The number of singular points (equilibrium solutions) of the OΔE and ODE must be the same. It should be indicated that a ΔE model can have more singular points than the ODE. This can lead to numerical instabilities.

Rule 4b. The stability properties of the singular points of the OΔE must be the same as the corresponding singular points of the ODE. Violation of this rule may lead to chaotic behavior (Ushiki, 1982).

Rule 5. Special or particular solutions of the OΔE should correspond to special or particular solutions of the ODE. In fact, they should have the "same general solution" as defined above.

PARTIAL DIFFERENTIAL EQUATIONS

The above rules have been presented for ODE's. However, they may also be applied to the construction of ΔE models of partial differential equations (PDE). "Exact difference schemes" may not exist for PDE's. This is a consequence of the fact that the concept of a general solution to PDE's is ambiguous. We do expect the existence of "exact difference schemes" for special classes of PDE's (Mickens, 1984).

As an illustration of the modeling process, consider the nonlinear diffusion equation

$$u_t = uu_{xx}, \quad u = u(x,t), \tag{19}$$

which has the following special solution

$$u^{(s)} = \frac{(\frac{\alpha}{2})x^2 + \beta_1 x + \beta_2}{\alpha_1 - \alpha t}, \tag{20}$$

where $(\alpha,\alpha_1,\beta_1,\beta_2)$ are arbitrary constants. Equation (19) can be modeled by the following explicit difference scheme

$$\frac{u_m^{n+1}-u_m^n}{\Delta t} = u_m^{n+1}\left[\frac{u_{m+1}^n-2u_m^n+u_{m-1}^n}{(\Delta x)^2}\right], \tag{21}$$

where $t_n = (\Delta t)n$ and $x_m = (\Delta x)m$. An easy calculation, using the method of separation of variables, shows that Eq. (21) has also the special solution given by $u_m^n = u^{(s)}[(\Delta x)m,(\Delta t)n]$. Note that this ΔE model satisfies all the modeling rules of the previous section. While we do not expect Eq. (21) to be an exact difference scheme for Eq. (19), it clearly is better than what would be obtained using conventional techniques (Richtmyer and Morton, 1967).

It should be indicated that Δt and Δx in Eq. (21) are not related to each other. However, in general, for PDE's, this will not be the case, i.e., a functional relationship will hold between the various step-sizes (Mickens, 1984).

CONCLUSION

The major advantage of obtaining exact ΔE models of DE's is that the usual problems relating to convergence, stability and consistency do not arise. In the absence of procedures for constructing exact difference schemes, the use of the above stated modeling rules will certainly lead to ΔE's that have a number of desireable properties which would not be expected to hold true for the usual modeling techniques. A very important area where these procedures might be applied is to nonlinear PDE's which have soliton solutions (Drazin, 1983).

REFERENCES

Drazin, P. G. (1983). Solitons. Cambridge University Press, London.

Jordan, D. W. and P. Smith (1977). Nonlinear Ordinary Differential Equations. Clarendon Press, Oxford.

Mickens, R. E. (1981). Nonlinear Oscillations. Cambridge University Press, London.

Mickens, R. E. (1984). Difference equation models of differential equations having zero local truncation errors. In I. W. Knowles and R. T. Lewis (Eds.), Differential Equations. North-Holland, Amsterdam, pp. 445-449.

Nayfeh, A. H. (1973). Perturbation Methods. Wiley, New York.

Potter, D. (1973). Computational Physics. Wiley, New York.

Potts, R. B. (1982a). Differential and difference equations. Am. Math. Mon., 89, 402-407.

Potts, R. B. (1982b). Best difference equation approximation to Duffing's equation. J. Austral. Math. Soc. Ser. B, 23, 349-356.

Potts, R. B. (1987). Weierstrass elliptic difference equations. Bull. Austral. Math. Soc., 35, 43-48.

Nemytski, V. V. and V. V. Stepanov (1969). Qualitative Theory of Differential Equations. Princeton University Press; Princeton, NJ.

Richtmyer, R. D. and K. W. Morton (1967). Difference Methods for Initial-Value Problems, 2nd ed. Wiley-Interscience, New York.

Ushiki, S. (1982). Central difference scheme and chaos. Physica, D4, 407-424.