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CONSTRUCTION OF STABLE EXPLICIT FINITE-DIFFERENCE SCHEMES FOR SCHRÖDINGER TYPE DIFFERENTIAL EQUATIONS

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ABSTRACT

A family of conditionally stable, forward Euler finite-difference equations can be constructed for the simplest equation of Schrödinger type, namely $u_t = iu_{xx}$. Generalization of this result to physically realistic Schrödinger type equations is presented.

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Introduction

Discrete finite-difference models of differential equations have been a traditional and popular technique for obtaining numerical solutions of both ordinary and partial differential equations [1,2]. An essential component of this procedure is the replacement of the derivative by its discrete analogue based on the definition of the derivative as a limit process; that is

$$\frac{dx}{dt} = \lim_{h \to 0} \frac{x(t+h) - x(t)}{h}, \tag{1}$$

and

$$\frac{dx}{dt} \to \frac{x_{k+1} - x_k}{h}, \tag{2}$$

where x_k is an approximation to $x(t_k)$ with $t_k = hk$. However, more general definitions of the derivative can be defined. As an example consider

$$\frac{dx}{dt} = \lim_{h \to 0} \frac{x(t+h) - x(t)}{\phi(h)}, \tag{3}$$

where $\phi(h)$ has the property

$$\phi(h) = h + 0(h^2). \tag{4}$$

Note that for this case the discrete replacement for the derivative is

$$\frac{dx}{dt} \to \frac{x_{k+1} - x_k}{\phi(h)}, \tag{5}$$

which, in general, differs from Eq. (2) for finite values of the step-size h.

The major implication of the above remarks is that new discrete models of differential equations can be constructed based on Eq. (3). These models have the potential for providing solutions that arise when the conventional discrete derivation of Eq. (2) is used.

As an illustration, consider the differential equation

$$\frac{dx}{dt} = i\lambda x, \qquad x(t_0) = x_0, \qquad \lambda = \text{real parameter}, \tag{6}$$

with solution

$$x(t) = x_0 \ \exp[\, i\lambda\,(t - t_0)\,]. \tag{7}$$

Application of conventional procedures [1] gives, for example, the finite-difference scheme

$$\frac{x_{k+1} - x_k}{h} = i\lambda x_k. \tag{8}$$

In contrast, consider the following <u>exact scheme</u> [3]

$$\frac{x_{k+1} - x_k}{\phi(h)} = i\lambda x_k, \quad x_0 = \text{given}, \tag{9}$$

where

$$\phi(h) = \frac{e^{i\lambda h} - 1}{i\lambda}. \tag{10}$$

An easy and direct calculation [4] shows that for Eqs. (6) and (8), we have for their solutions $x(t_k) \neq x_k$, while for Eqs. (6) and (9), $x(t_k) = x_k$ for all step-sizes h. Also, from Eq. (10), we obtain

$$\phi(h) = h + i\lambda h^2 + 0(h^3). \tag{11}$$

Consider the simplest Schrödinger-type equation

$$u_t = iu_{xx}. \tag{12}$$

Conventional finite-differences, using a forward Euler replacement for the time-derivative, give a scheme that is unconditionally unstable [5]. We now show how conditionally stable schemes can be constructed.

To proceed, based on the discussion presented earlier, we construct the following finite-difference scheme

$$\frac{u_m^{n+1} - u_m^n}{i\phi_1(\Delta t,\lambda)} = \frac{u_{m+1} - 2u_m^n + u_{m-1}^n}{\phi_2\,(\Delta x,\lambda)} \tag{13}$$

where the "denominator functions" have the properties

$$\phi_1(\Delta t, \lambda) = \Delta t + i\lambda(\Delta t)^2 + 0[(\Delta t)^3] \tag{14a}$$

$$\phi_2\,(\Delta x, t) = (\Delta x)^2 + 0[(\Delta x)^3] \tag{14b}$$

and λ, for the moment, is an unspecified parameter. Defining $R(\Delta t, \Delta x, \lambda)$ as

$$R \equiv \frac{i\phi_1(\Delta t, \lambda)}{\phi_2(\Delta x, \lambda)} = R_1(\Delta t, \Delta x, \lambda) + iR_2\,(\Delta t, \Delta x, \lambda) \tag{15}$$

we can rewrite Eq. (13) in the form

$$u_m^{n+1} = Ru_{m+1}^n + (1-2R)\,u_m^n + Ru_m^n.$$

The substitution of a typical Fourier mode

$$u_m^n = C(n)\exp[\,i\omega(\Delta x)m], \tag{17}$$

into Eq. (16) and requiring the C(n) be bounded allows the determination of the stability properties. (This concept of stability is called "practical stability" [5,6].) A straight-forward calculation shows that Eq. (16) is stable if the following condition is satisfied.

$$(R_1 - \frac{1}{4})^2 + (R_2)^2 \le \frac{1}{16}\,. \tag{18}$$

This relation has the interesting geometric interpretation: In the (R_1,R_2) plane, Eq. (16) is stable for points on and inside the circle of radius 0.25 centered at (0.25, 0). We will refer to the inequality of Eq. (18) as the circle condition.

For a given application, the following procedure is to be followed:

a) Select denominator functions with the properties given in Eqs. (14) and calculate R in Eq. (15).

b) Choose a point $(\bar{R}_1, \bar{R}_2)$ consistent with the circle condition of Eq. (18).

c) Determine $R_1(\Delta t, \Delta x, \lambda)$ and $R_2(\Delta t, \Delta x, \lambda)$ from Eq. (15) and set them equal, respectively to $\bar{R}_1$ and $\bar{R}_2$, i.e.,

$$R_1(\Delta t, \Delta x, \lambda) = \bar{R}_1, \quad \bar{R}_2(\Delta t, \Delta x, \lambda) = \bar{R}_2. \tag{19}$$

d) Select a value for the space-step, Δx, and solve the two relations of Eq. (19) for Δt and λ in terms of Δx. Doing this gives

$$\Delta t = f_1(\Delta x), \quad \lambda = f_2(\Delta x). \tag{20}$$

Thus, the selection of the point $(\bar{R}_1, \bar{R}_2)$, satisfying the circle condition and the relations of Eq. (20), defines completely the finite-difference scheme of Eq. (16).

As an example, consider the following denominator functions

$$\phi_1 = \Delta t + i\lambda(\Delta t)^2, \quad \phi_2 = (\Delta x)^2, \tag{21}$$

with

$$\bar{R} = \frac{1+i}{4}. \tag{22}$$

The following results are easily obtained

$$\Delta t = \frac{(\Delta x)^2}{4}, \quad \lambda = -\left[\frac{4}{(\Delta x)^2}\right], \quad \phi_1 = \frac{1-i}{4}. \tag{23}$$

and

$$u_m^{n+1} = \left(\frac{1+i}{4}\right)[u_{m+1}^n + u_{m-1}^n] + \left(\frac{1-i}{2}\right)u_m^n. \tag{24}$$

Note that everything can be expressed in terms of Δx, the space step-size; its value can be selected as desired.

A second, nontrivial example is the nonlinear Schrödinger equation

$$u_t = iu_{xx} + |u|^2u. \tag{25}$$

A finite-difference scheme that embodies the work of this paper and also uses the nonlocal modeling of the nonlinear term [3] is

$$\frac{u_m^{n+1} - u_m^n}{\phi_1} = i\left[\frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{\phi_2}\right]$$
$$+\left[\frac{u_{m+1}^n + u_{m-1}^n}{2}\right]^*\left[\frac{u_{m+1}^n + u_{m-1}^n}{2}\right]u_m^{n+1}, \tag{26}$$

where the star (*) denotes complex conjugation, and the denominator functions $\phi_1(\Delta t, \lambda)$ and $\phi_2(\Delta x, \lambda)$ satisfy the conditions of Eqs. (14). Note that Eq. (20) is an explicit finite-difference scheme.

In summary, we have presented a new procedure to construct explicit finite-difference schemes for Schrödinger type partial differential equations. In general, we expect these schemes to be conditionally stable. This paper summarizes research that has already been published in Physics Review A, June 1989 and in the "Proceedings of the 2nd IMAC Conference on Computational Acoustics."

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