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Short Communication

A numerical integration technique for conservative oscillators combining nonstandard finite-difference methods with a Hamilton's principle

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Abstract

Nonstandard finite difference schemes are constructed for several important conservative oscillators. These procedures combine the nonstandard methods of Mickens (J. Sound Vib. 240 (2001) 587) with a discrete Hamilton's principle.

An ordinary differential equation modeling many of the important features of nonlinear oscillations is [1]

$$\ddot{x} + \omega^2 x + fx^2 + gx^3 = 0, \tag{1}$$

where (ω, f, g) are constant parameters. While analytical results based on perturbation methods provide useful insights into the properties of the solutions for the case where the nonlinear terms are small [2], numerical procedures are generally required when the nonlinear terms are large [3]. Previous work by Mickens [4], which was based on the use of a discrete energy function [5], provided a finite-difference model for Eq. (1) that could be applied to the determination of numerical solutions. The major task of this letter is to generalize these results [4] by combining nonstandard finite-difference methods with a particular discretization of Hamilton's principle to

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obtain a new discrete finite-difference scheme for Eq. (1) that also turns out to be a symplectic method [6]. (A concise introduction to the relevant references and related background information on the general theory of symplectic integrators is given in Ref. [6, Chapter 6].)

To illustrate the general procedure, consider the simple harmonic oscillator (SHO)

$$\ddot{x} + x = 0, \tag{2}$$

which has the energy function [1]

$$E(x, \dot{x}) = \left(\frac{1}{2}\right)\dot{x}^2 + \left(\frac{1}{2}\right)x^2 = \text{constant}. \tag{3}$$

The corresponding Lagrange function is [1]

$$L(x, \dot{x}) = \left(\frac{1}{2}\right)\dot{x}^2 - \left(\frac{1}{2}\right)x^2, \tag{4}$$

which can be discretized as

$$L(x, \dot{x}) \to L(x_n, x_{n+1}), \tag{5}$$

where

$$t \to t_n = hn, \quad h = \Delta t; \quad x(t) \to x_n \tag{6}$$

and $L(x_n, x_{n+1})$ is given by the expression

$$L(x_n, x_{n+1}) = \left(\frac{1}{2}\right)\left(\frac{x_{n+1} - x_n}{\phi}\right)^2 - \left(\frac{1}{2}\right)\left[\frac{ax_{n+1}^2 + bx_{n+1}x_n + cx_n^2}{a+b+c}\right], \tag{7}$$

where (a, b, c) are positive parameters and ϕ is a function of h. Previous work [5] has shown that $L(x_n, x_{n+1})$ must satisfy the relation

$$L(x_n, x_{n+1}) = L(x_{n+1}, x_n). \tag{8}$$

This result implies that $a = c$. To proceed, the discrete modified Lagrange function must be introduced; it is given by [6]

$$L_h(x_n, x_{n+1}) = hL(x_n, x_{n+1}), \tag{9}$$

where $h = \Delta t$ is the time step-size. Note that the discrete expression for x^2, i.e.,

$$x^2 \to \frac{ax_{n+1}^2 + bx_{n+1}x_n + ax_n^2}{2a+b} \tag{10}$$

is the most general one that can be written down which satisfies the requirement given by Eq. (8). Putting all this together gives for $L_h(x_n, x_{n+1})$ the result

$$L_h(x_n, x_{n+1}) = \left(\frac{h}{2}\right)\left(\frac{x_{n+1} - x_n}{\phi}\right)^2 - \left(\frac{h}{2}\right)\left[\frac{ax_{n+1}^2 + bx_{n+1}x_n + ax_n^2}{2a+b}\right], \tag{11}$$

where the denominator function [3], $\phi(h)$, has the property

$$\phi(h) = h + O(h^2). \tag{12}$$

The equation of motion for x_n follows from the discrete Euler–Lagrange equations [6]

$$\frac{\partial L_h(x_{n-1}, x_n)}{\partial x_n} + \frac{\partial L_h(x_n, x_{n+1})}{\partial x_n} = 0. \tag{13}$$

Substituting Eq. (11) into this relation gives

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\phi^2} + \frac{bx_{n+1} + 4ax_n + bx_{n-1}}{2(2a+b)} = 0, \tag{14}$$

which is the discrete finite-difference model for the SHO given by Eq. (2). Observe that it is a linear, second-order difference equation and the linear x term, in Eq. (2), is modeled nonlocally, i.e.,

$$x \to \frac{bx_{n+1} + 4ax_n + bx_{n-1}}{2(2a+b)}. \tag{15}$$

Also, note that this expression is invariant under the substitution

$$(n+1) \leftrightarrow (n-1). \tag{16}$$

This is the discrete version [5] of the time-reversal property of Eq. (2), i.e., Eq. (2) is invariant under $t \to (-t)$.

The corresponding discrete momentum is given by [6]

$$p_n = -\frac{\partial L_h(x_n, x_{n+1})}{\partial x_n}. \tag{17}$$

Using L_h from Eq. (11) gives

$$p_n = \frac{x_{n+1} - x_n}{D(h)} + \left(\frac{h}{2}\right)\left[\frac{bx_{n+1} + 2ax_n}{2a+b}\right], \tag{18}$$

where

$$D(h) = \frac{\phi^2(h)}{h}. \tag{19}$$

(For the case where $\phi(h) = h$, then $D(h) = h$.) For standard numerical integration schemes, the momentum is expressed by the first term in Eq. (18), namely, by a forward-Euler discrete representation. Our nonstandard finite difference scheme combined with the symplectic Hamilton principle gives a value for p_n that is modified by the presence of a term of order h. Thus, in the limit $h \to 0$, this expression reduces to the usual definition of the momentum. Also, Eq. (19) shows that the denominator function [3] appearing in the discrete momentum is not, in general, $\phi(h)$, but $D(h)$.

Returning to Eq. (1), an easy calculation gives the energy function [1]

$$E(x, \dot{x}) = \left(\frac{1}{2}\right)\dot{x}^2 + \left(\frac{\omega^2}{2}\right)x^2 + \left(\frac{f}{3}\right)x^3 + \left(\frac{g}{4}\right)x^4 = \text{constant}. \tag{20}$$

Likewise, the Lagrange function is [1]

$$L(x,\dot{x}) = \left(\frac{1}{2}\right)\dot{x}^2 - \left(\frac{\omega^2}{2}\right)x^2 - \left(\frac{f}{3}\right)x^3 - \left(\frac{g}{4}\right)x^4. \tag{21}$$

From this latter expression a general, invariant under $n \leftrightarrow (n+1)$, discrete Lagrange function can be constructed; it is

$$\begin{aligned} L(x_n, x_{n+1}) = {} & \left(\frac{1}{2}\right)\left(\frac{x_{n+1}-x_n}{\phi}\right)^2 - \left(\frac{\omega^2}{2}\right)\left[\frac{a(x_{n+1}^2+x_n^2)+bx_{n+1}x_n}{2a+b}\right] \\ & - \left(\frac{f}{3}\right)\left[\frac{a_1(x_{n+1}^3+x_n^3)+b_1(x_{n+1}^2x_n+x_{n+1}x_n^2)}{2(a_1+b_1)}\right] \\ & - \left(\frac{g}{4}\right)\left[\frac{a_2(x_{n+1}^4+x_n^4)+b_2(x_{n+1}^3x_n+x_{n+1}x_n^3)+c_2x_{n+1}^2x_n^2}{2a_2+2b_2+c_2}\right], \end{aligned} \tag{22}$$

where $(a, b, a_1, b_1, a_2, b_2, c_2)$ are nonnegative parameters. Applying Eqs. (9) and (13), the discrete equation of motion can be determined and is given by

$$\begin{aligned} & \frac{x_{n+1}-2x_n+x_{n-1}}{\phi^2} + \omega^2\left[\frac{4ax_n+b(x_{n+1}+x_{n-1})}{2(2a+b)}\right] \\ & + f\left\{\frac{6a_1x_n^2+b_1[x_{n+1}^2+x_{n-1}^2+2x_n(x_{n+1}+x_{n-1})]}{6(a_1+b_1)}\right\} \\ & + g\left\{\frac{8a_2x_n^3+b_2[x_{n+1}^3+3x_n^2(x_{n+1}+x_{n-1})+x_{n-1}^3]+2c_2x_n(x_{n+1}^2+x_{n-1}^2)}{4(2a_2+2b_2+c_2)}\right\} = 0. \end{aligned} \tag{23}$$

Likewise, the discrete momentum is determined by using Eqs. (8), (17), and (22); it is

$$\begin{aligned} p_n = {} & \frac{x_{n+1}-x_n}{D(h)} - \left(\frac{\omega^2 h}{2}\right)\left[\frac{2ax_n+bx_{n+1}}{2a+b}\right] - \left(\frac{fh}{3}\right)\left[\frac{3a_1x_n^2+b_1(x_{n+1}+2x_n)x_{n+1}}{2(a_1+b_1)}\right] \\ & - \left(\frac{gh}{4}\right)\left[\frac{4a_2x_n^3+b_2(x_{n+1}^2+3x_n^2)x_{n+1}}{2a_2+2b_2+c_2}\right], \end{aligned} \tag{24}$$

where $D(h)$ is that of Eq. (19). Again, just as for the case of the SHO, both the equation of motion and the momentum display a much more complex structure than discrete schemes based on standard procedures. For example, the use of a forward-Euler scheme for the discrete derivative and local forms for the other terms provides the following forms for the determination of x_n and p_n [3]:

$$\frac{x_{n+1}-2x_n+x_{n-1}}{h^2} + \omega^2 x_n + fx_n^2 + gx_n^3 = 0, \tag{25}$$

$$p_n = \frac{x_{n+1}-x_n}{h}. \tag{26}$$

The use of nonstandard finite-difference techniques without the joint application of the discrete Hamilton's principle, as presented in Ref. [6], gives for Eq. (1), the discretization

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\phi^2} + \omega^2 x_n + f\left(\frac{x_{n+1} + x_n + x_{n-1}}{3}\right)x_n + g\left(\frac{x_{n+1} + x_{n-1}}{2}\right)x_n^2 = 0, \tag{27}$$

$$p_n = \frac{x_{n+1} - x_n}{\phi}. \tag{28}$$

It is clearly seen that combining the nonstandard method with a discrete Hamilton principle, which is symplectic, gives a much more complex equation of motion and expression for the momentum. Also, note that the discretizations of Eqs. (25) and (27) are linear in x_{n+1} and thus are explicit, while the second-order, nonlinear finite-difference representation of Eq. (23) is implicit.

These methods can also be generalized to systems of coupled nonlinear oscillators. In general, such derived schemes will be implicit in nature and have complex expressions for the various momentum functions in comparison to the usual methods. An example illustrating this behavior is the Hénon–Heiles system [7,8]. The Lagrange function is

$$L(x, \dot{x}; y, \dot{y}) = \left(\frac{1}{2}\right)(\dot{x}^2 + \dot{y}^2) - \left(\frac{1}{2}\right)\left[x^2 + y^2 - \left(\frac{2}{3}\right)y^3\right] - x^2 y \tag{29}$$

and the equation of motion are

$$\ddot{x} + x + 2xy = 0, \quad \ddot{y} + y - y^2 + x^2 = 0. \tag{30}$$

Taking the discrete Lagrange function to be

$$\begin{aligned} L_h(x_n, x_{n+1}; y_n, y_{n+1}) = {} & \left(\frac{h}{2}\right)\left[\left(\frac{x_{n+1} - x_n}{\phi}\right)^2 + \left(\frac{y_{n+1} - y_n}{\phi}\right)^2\right] - \left(\frac{h}{2}\right)(x_{n+1}x_n + y_{n+1}y_n) \\ & + \left(\frac{h}{2}\right)\left(\frac{2}{3}\right)\left[\frac{y_{n+1}^2 y_n + y_{n+1} y_n^2}{2}\right] - \left(\frac{h}{2}\right)x_{n+1}x_n(y_{n+1} + y_n), \end{aligned} \tag{31}$$

the equations of motion for x_n and y_n can be determined from the expressions [6]

$$\frac{\partial L_h(x_{n-1}, x_n; y_n, y_{n-1})}{\partial x_n} + \frac{\partial L_h(x_n, y_{n+1}; y_n, y_{n+1})}{\partial x_n} = 0, \tag{32a}$$

$$\frac{\partial L_h(x_{n-1}, x_n; y_{n-1}, y_n)}{\partial y_n} + \frac{\partial L_h(x_n, x_{n+1}; y_n, y_{n+1})}{\partial y_n} = 0. \tag{32b}$$

From $L_h(x_n, x_{n+1}; y_n, y_{n-1})$ and these latter equations, a direct calculation gives

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\phi^2} + \left(\frac{x_{n+1} + x_{n-1}}{2}\right) + \left[x_{n+1}\left(\frac{y_{n+1} + y_n}{2}\right) + x_{n-1}\left(\frac{y_n + y_{n-1}}{2}\right)\right] = 0, \tag{33}$$

$$\begin{aligned} & \frac{y_{n+1} - 2y_n + y_{n-1}}{\phi^2} + \left(\frac{y_{n+1} + y_{n-1}}{2}\right) - \left[\frac{y_{n+1}^2 + 2y_n(y_{n+1} + y_{n-1}) + y_{n-1}^2}{6}\right] \\ & + \left(\frac{x_{n+1} + x_{n-1}}{2}\right)x_n = 0, \end{aligned} \tag{34}$$

where the corresponding momentum expressions are

$$p_n^{(x)} = \frac{x_{n+1} - x_n}{D(h)} + \left(\frac{h}{2}\right)(1 + y_{n+1} + y_n)x_{n+1}, \tag{35a}$$

$$p_n^{(y)} = \frac{y_{n+1} - y_n}{D(h)} + \left(\frac{h}{2}\right)\left\{\left[1 - \left(\frac{1}{3}\right)(y_{n+1} + 2y_n)\right]y_{n+1} + x_{n+1}x_n\right\}, \tag{35b}$$

and where $D(h)$ is the same as that of Eq. (19).

To summarize, the previous work of Mickens [4], using nonstandard finite difference methods, have been extended to include results on a symplectic integrator which comes from using a discretized Hamilton principle [6]. This procedure was illustrated by first applying it to the simple harmonic oscillator and then the general nonlinear conservative oscillator where the force function is cubic in the displacement. An additional application was to the Hénon–Heiles system. Finally, it should be noted that the major contribution of the nonstandard methods, as used by Mickens [3,4] in his work, is to provide a general methodology for the construction of improved discretized Lagrange functions.

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