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# A NON-STANDARD FINITE-DIFFERENCE SCHEME FOR CONSERVATIVE OSCILLATORS

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Many important dynamical systems can be modeled one-dimensional non-linear oscillators [1, 2]. For information on the properties of such systems, a variety of analytical methods exist which can be used to construct approximations to the periodic solutions [3, 4]. However, when very accurate solutions are needed, the usual practical procedure is to numerically integrate the equations of motion (EOM) [5, 6]. A major difficulty with numerical techniques is that they can give rise to numerical instabilities; these are solutions of the discrete equations, used for the numerical integration, that do not correspond to any solution of the differential equation [5, 6]. For conservative oscillators, numerical instabilities arise when the second order finite-difference schemes do not possess a discrete version of the first integral that exists for the EOM [7, 8]. This first integral, for conservative systems, is the energy function [2].

In an earlier paper [8], it was shown how to construct a discrete energy function such that the derived EOM provided an accurate discrete model of the original differential equation. However, this paper [8] only derived the EOM for a one-dimensional oscillator for which the potential energy was a quartic function of the dependent variable $x$, i.e.,

$$V(x) = a_0 + a_1 x + \frac{a_2 x^2}{2} + \frac{a_3 x^3}{3} + \frac{a_4 x^4}{4}, \tag{1}$$

where ($a_0$, $a_1$, $a_2$, $a_3$, $a_4$) are constants. The main purpose of this Letter is to generalize the results of Mickens [8] to the case where $V(x)$ is a general polynomial function of $x$ of $J$th degree, for arbitrary but finite integer $J$.

A conservative one-dimensional oscillator satisfies the following conservation law [2]:

$$E(x, x) = (\tfrac{1}{2})\dot{x}^2 + V(x) = \text{constant}, \tag{2}$$

where the constant is determined by the initial conditions, i.e., if $x(0) = x^{(0)}$ and $\dot{x}(0) = \dot{x}^{(0)}$; then

$$E(\dot{x}, x) = (\tfrac{1}{2})(\dot{x}^{(0)})^2 + V(x^{(0)}). \tag{3}$$

The EOM is obtained by taking the time-derivative of the energy function [2, 8],

$$\frac{\mathrm{d}E(\dot{x}, x)}{\mathrm{d}t} = \frac{\partial E}{\partial \dot{x}}\frac{\mathrm{d}\dot{x}}{\mathrm{d}t} + \frac{\partial E}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} = \dot{x}\left[\ddot{x} + \frac{\mathrm{d}V(x)}{\mathrm{d}x}\right] = 0 \tag{4}$$

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or

$$\ddot{x} + \frac{\mathrm{d}V(x)}{\mathrm{d}x} = 0. \tag{5}$$

Let $V(x)$ be a $J$th degree polynomial, written as

$$V(x) = \sum_{j=0}^{J} \frac{a_j x^j}{j}, \tag{6}$$

then equation (5) becomes

$$\ddot{x} + \sum_{j=1}^{J} a_j x^{j-1} = 0. \tag{7}$$

In Mickens [8], it was shown that a discrete energy function should be constructed such that it is a function only of $x_k$ and $x_{k-1}$, and be invariant under the interchange: $x_k \leftrightarrow x_{k-1}$, i.e.,

$$E(\dot{x}, x) \to \bar{E}(x_k, x_{k-1}), \tag{8}$$

where

$$\bar{E}(x_k, x_{k-1}) = \bar{E}(x_{k-1}, x_k), \tag{9}$$

$$t \to t_k = hk, \qquad x(t_k) \to x_k, \qquad h = \Delta t, \tag{10}$$

and the following choice is made for the discrete representation of the derivative:

$$\dot{x} \to \frac{x_k - x_{k-1}}{\phi(h)}, \tag{11}$$

and $\phi(h)$, the denominator function, is only required to have the property [5]

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

The question now arises as what discrete representation should be used for the terms $x^j$ in the potential energy function given in equation (6)? In the work to follow, only the *minimalist* representation will be used, i.e., the discrete model for $x^j$ will consist of one term, if $j$ = even, or two terms, if $j$ = odd. While other possibilities exist, this selection gives the results for discrete EOM which are in agreement with the mathematical structure of the original differential equations. First, note that for the constant and linear terms in $V(x)$, the discrete models are

$$a_0 + a_1 x \to a_0 + \frac{a_1(x_k + x_{k-1})}{2}. \tag{13}$$

Likewise, using the result in equation (11) gives for the kinetic energy term the representation

$$(\tfrac{1}{2})\dot{x}^2 \to (\tfrac{1}{2})\left(\frac{x_k - x_{k-1}}{\phi}\right)^2. \tag{14}$$

Consider now the case where $j$ = even. A minimalist representation for $x^j$ is ($j = 2m$)

$$j = \text{even:}\ \frac{x^j}{j} = \frac{x^m x^m}{2m} \to \frac{(x_k)^m (x_{k-1})^m}{2m}. \tag{15}$$

For $j$ = odd, then the minimalist representation takes the form ($j = 2m + 1$)

$$j = \text{odd:}\ \frac{x^j}{j} = \frac{x^{m+1}x^m + x^m x^{m+1}}{2(2m+1)} \to \frac{(x_k)^{m+1}(x_{k-1})^m + (x_k)^m (x_{k-1})^{m+1}}{2(2m+1)}. \tag{16}$$

The discrete model of the potential energy consequently can be written as

$$V(x) \to \bar{V}(x_k, x_{k-1}) = \sum_{j=0}^{J} \frac{a_j [x^j]_k}{j}, \tag{17}$$

where the symbol $[x^j]_k$ is either the result from equations (15) or (16) depending as to whether $j$ = even or odd, with $j \geqslant 2$.

Using equations (14) and (17), the following discrete energy function is obtained:

$$\bar{E}(x_k, x_{k-1}) = (\tfrac{1}{2}) \left( \frac{x_k - x_{k-1}}{\phi} \right)^2 + \bar{V}(x_k, x_{k-1}). \tag{18}$$

Note that by the method of its construction the discrete energy function automatically satisfies the condition given by equation (9). The discrete EOM is determined by applying the operator $\Delta$ as defined as

$$\Delta f_k \equiv f_{k+1} - f_k, \tag{19}$$

to $\bar{E}(x_k, x_{k-1})$, i.e.,

$$\Delta \bar{E}(x_k, x_{k-1}) = 0. \tag{20}$$

For the discrete kinetic energy, it follows that

$$\Delta \left[ (\tfrac{1}{2}) \left( \frac{x_k - x_{k-1}}{2} \right)^2 \right] = \left( \frac{x_{k+1} - x_{k-1}}{2} \right) \left[ \frac{x_{k+1} - 2x_k + x_{k-1}}{\phi^2} \right] \tag{21}$$

and

$$\Delta \left[ a_0 + a_1 \frac{(x_k + x_{k-1})}{2} \right] = a_1 \left( \frac{a_{k+1} - x_{k-1}}{2} \right). \tag{22}$$

For the various other potential energy terms, the following results are obtained after a certain amount of algebraic manipulations:

$j$ = even = $2m$

$$\Delta \left[ \frac{(x_k)^m (x_{k-1})^m}{2m} \right] = \left( \frac{x_{k+1} - x_{k-1}}{2} \right) (x_k)^m \times \left[ \frac{(x_{k+1})^{m-1} + (x_{k+1})^{m-2} x_{k-1} + \cdots + x_{k+1}(x_{k-1})^{m-2} + (x_{k-1})^{m}}{m} \right]. \tag{23}$$

$j = \text{odd} = 2m+1$

$$\Delta\left[\frac{(x_k)^{m+1}(x_{k-1})^m + (x_k)^m(x_{k-1})^{m+1}}{2(2m+1)}\right] = \left(\frac{x_{k+1}-x_{k-1}}{2}\right)(x_k)^m$$
$$\times\left\{\frac{[(x_{k+1})^m + (x_{k+1})^{m-1}x_{k-1} + \cdots + (x_{k+1})^m] + x_k[(x_{k+1})^{m-1} + \cdots + (x_{k-1})^{m-1}]}{2m+1}\right].\tag{24}$$

It should be pointed out that the major bracketed expressions, respectively, on the right-hand sides of equations (22) and (23), contain $m$ and $2m+1$ terms. This means that in the limits: $h \to 0$, $k \to \infty$, $hk = t = \text{fixed}$, these expressions reduce, respectively, to the correct values of $x^{m-1}$ and $x^m$.

An important observation is that the given results in equations (21)–(24), each term, on the right-hand side, contains the factor $(x_{k+1} - x_{k-1})/2$. As a consequence, the discrete EOM can be obtained from the expression

$$\Delta\bar{E}(x_k, x_{k-1}) = \left(\frac{x_{k+1}-x_{k-1}}{2}\right)H(x_{k+1}, x_k, x_{k-1}) = 0, \tag{25}$$

where

$$H(x_{k+1}, x_k, x_{k-1}) = 0 \tag{26}$$

is the required EOM. Further, it clearly follows that $H(x_{k+1}, x_k, x_{k-1})$ is invariant under the interchange $(k+1)\leftrightarrow(k-1)$. This discrete symmetry is equivalent to the corresponding invariance under time-reversal, $t \to -t$, for the original differential equation or its first integral, the energy functions. Thus, the above method for constructing a discrete energy function and its associated EOM mirrors exactly the properties of the differential equation. Thus, the usual numerical instabilities are not expected to occur [5, 7, 8] in the finite-difference scheme given by equation (26).

Several comments are in order at this point. (1) For $J \geqslant 5$, the finite-difference scheme is implicit. This means that in equation (26), $x_{k+1}$ satisfies an algebraic equation of at least degree two. (2) For $J \leqslant 4$, the above minimalist way of constructing the discrete representations of the polynomial terms in the potential energy function leads to an EOM in which $x_{k+1}$ appears linearly in each term for which it occurs. This means that $x_{k+1}$ can be explicitly solved for (by hand) and directly expressed in terms of $x_k$ and $x_{k-1}$. (3) For a particular nonlinear oscillator differential equation, a time step-size has to be selected after the discrete model has been constructed. It should be kept in mind that the maximum step-size is determined by physical considerations, i.e., it must be chosen such that its value is "small" compared to the period of the oscillation. For most problems involving one-dimensional oscillations, excellent estimates can be obtained for the period by use of dimensional analysis [1, 9] or the method of harmonic balance [4].

Finally, to illustrate the method and to extend the work of Mickens [8], results are presented for the quintet potential energy function. The energy function and EOM are

$$E(\dot{x}, x) = (\tfrac{1}{2})\dot{x}^2 + a_1 x + \frac{a_2 x^2}{2} + \frac{a_3 x^3}{3} + \frac{a_4 x^4}{4} + \frac{a_5 x^5}{5}, \tag{27}$$

$$\dot{x} + a_1 + a_2 x + a_3 x^2 + a_4 x^3 + a_5 x^4 = 0. \tag{28}$$

The corresponding discrete representations are

$$\bar{E}(x_k, x_{k-1}) = (\tfrac{1}{2})\left(\frac{x_k - x_{k-1}}{2}\right)^2 + a_1\left(\frac{x_k + x_{k-1}}{2}\right) + a_2\left(\frac{x_k x_{k-1}}{2}\right)$$
$$+ \left(\frac{a_3}{3}\right)\left[\frac{(x_k)^2 x_{k-1} + x_k(x_{k-1})^2}{2}\right] + \left(\frac{a^4}{4}\right)(x_k)^2(x_{k-1})^2$$
$$+ \left(\frac{a_5}{5}\right)\left[\frac{(x_k)^3(x_{k-1})^2 + (x_k)^2(x_{k-1})^3}{2}\right], \tag{29}$$

and

$$\frac{x_{k+1} - 2x_k + x_{k-1}}{\phi^2} + a_1 + a_2 x_k + a_3\left(\frac{x_{k+1} + x_k + x_{k-1}}{3}\right)x_k$$
$$+ a_4\left(\frac{x_{k+1} + x_{k-1}}{2}\right)x_k^2$$
$$+ a_5\left[\frac{(x_{k+1})^2 + x_{k+1}x_{k-1} + (x_{k-1})^2 + x_k(x_{k+1} + x_{k-1})}{5}\right]x_k^2. \tag{30}$$

As expected, the scheme is implicit, with $x_{k+1}$ appearing as a square in the term having $a_5$ as a coefficient.

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