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Note

An Explicit Energy-Conserving Numerical Method for Equations of the Form $d^2x/dt^2 = f(x)$

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Physics is characterized by conservation laws and by symmetry [2]. Therefore the methods in computational physics should be conservative. Unfortunately most methods in the literature are not totally energy conserving, even for the simplest initial-value problem:

$$d^2x/dt^2 = f(x); \qquad x(0) = \alpha,\ dx/dt|_{t=0} = \beta. \tag{1.1}$$

The question is raised first by D. Greenspan [1]. Introducing a function $\phi(x)$:

$$-d\phi/dx = f(x). \tag{1.2}$$

The energy conservation equation is expressed as

$$\tfrac{1}{2}(dx/dt)^2 + \phi(x) = \tfrac{1}{2}\beta^2 + \phi(\alpha). \tag{1.3}$$

In [1], Greenspan developed two methods for the problem (1.1) with the conservation relation (1.3) and gave numerical examples. But the two methods are implicit forms and require iterative calculations. Conditions should be put in order to guarantee the convergence of the iterative process. The methods also are not easy to extend to systems of particles, because the iterative sequences increase exponentially. These have been pointed out also in [1]. In this paper we suggest an explicit and simple numerical method to overcome these different difficulties.

2. The Explicit Energy-Conserving Method

We propose an explicit scheme satisfying (1.3) under the condition (1.2) for the problem (1.1) as

$$Xn+1 = Xn + \frac{\Delta t}{1!}(dx/dt)\,n + \frac{(\Delta t)^2}{2!}f(Xn) \tag{2.1}$$

$$(dx'/dt)\,n+1 = (dx/dt)\,n + \frac{\Delta t}{1!}f(Xn) \tag{2.2}$$

$$(dx/dt)\,n+1 = (\text{sgn}(dx'/dt)\,n+1)\left|\sqrt{\beta^2 + 2\phi(\alpha) - 2\phi(Xn+1)}\right| \tag{2.3}$$

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where the signature function is defined by

$$\operatorname{sgn}(dx'/dt)\, n+1 = \begin{cases} +1 & \text{when} \quad (dx'/dt)\, n+1 > 0 \\ -1 & \text{when} \quad (dx'/dt)\, n+1 < 0, \end{cases} \tag{2.4}$$

for the case

$$\beta^2 + 2\phi(\alpha) - 2\phi(Xn+1) \geqslant 0$$

and

$$(\operatorname{sgn}(dx'/dt)\, n+1)(\operatorname{sgn}(dx'/dt)\, n) > 0.$$

For the special case $\beta^2 + 2\phi(\alpha) - 2\phi(Xn+1) < 0$ or $\operatorname{sgn}(dx'dt)\, n+1 = 0$ or $(\operatorname{sgn}(dx'/dt)\, n+1)(\operatorname{sgn}(dx'/dt)\, n) < 0$. Then we should choose Δt such that

$$\beta^2 + 2\phi(\alpha) - 2\phi(Xn+1) = 0; \tag{2.2$'$}$$

and then for this Δt and $Xn+1$, we have

$$(dx/dt)\, n+1 = 0. \tag{2.3$'$}$$

The initial values are

$$X_0 = \alpha \qquad \text{and} \qquad (dx/dt)_0 = \beta. \tag{2.5}$$

Rewriting Eq. (2.3), we can get the exact relation

$$\tfrac{1}{2}(dx/dt)^2 n+1 + \phi(Xn+1) = \tfrac{1}{2}\beta^2 + \phi(\alpha). \tag{2.6}$$

Equation (2.6) is the discrete scheme of the energy conserving relation (1.3), because $(dx/dt)n+1$ in (2.6) can take two values, so we use Eq. (2.3) to fix the sign of $(dx/dt)\, n+1$ as that of $(dx'/dt)\, n+1$.

The scheme (2.1)–(2.3) is clearly direct, simple, and above all, totally energy conserving.

3. Computational Examples

We shall use our method to calculate two examples given in [1] and compare the results. The computer used here is the TI-59.

Example 1. $d^2x/dt^2 = x^2$; $X(0) = 1$; $(dx/dt)_0 = 1$. Let $\phi(x) = -X^3/3$, so we have the total energy

$$E_0 = \tfrac{1}{2} + (-\tfrac{1}{3}) = \tfrac{1}{6}.$$

The system of difference equations is then

$$Xn+1 = Xn + \frac{\Delta t}{1!}(dx/dt)\,n + \frac{(\Delta t)^2}{2!}(X_n^2),$$

$$(dx'/dt)\,n+1 = (dx/dt)\,n + (\Delta t)\,Xn^2,$$

$$(dx/dt)\,n+1 = \mathrm{sgn}(dx'/dt)\,n+1\,\left|\sqrt{\tfrac{1}{3} + (2/3)\,X_{n+1}^3}\right|.$$

Take $\Delta t = 0.01$, for $t = 0$ to 0.5, the results compared with [1] are as follows:

	t	x	dx/dt	E
This method	0.5	1.680501387	1.870094225	0.1666666667
Method 1 in [1]	0.5	1.6805618966	1.8701856026	0.166667
Method 2 in [1]	0.5	1.6805416400	1.8701550119	0.166667

EXAMPLE 2. $d^2x/dt^2 = -\sin x$, $x(0) = \pi/2$, $(dx/dt)_0 = 0$. Take $\phi(x) = -\cos x$, so we have the total energy:

$$E_0 = 0 + 0 = 0.$$

The system of difference equations is

$$Xn+1 = Xn + (\Delta t)(dx/dt)\,n - \frac{(\Delta t)^2}{2}\sin(Xn),$$

$$(dx'/dt)\,n+1 = (dx/dt)\,n - (\Delta t)\sin(Xn),$$

$$(dx/dt)\,n+1 = (\mathrm{sgn}(dx'/dt)\,n+1)\left|\sqrt{2\cos(Xn+1)}\right|.$$

Take $\Delta t = 0.01$ for $t = 0$ to 0.5, the results compared with [1] are as follows:

	+	×	dx/dt	E
This method	0.5	1.445861213	−0.4992200973	0.000000000
Method 1 in [1]	0.5	1.4458614667	−0.4992195939	0.000000

This method has been extended to the three-body problem by conservation of energy; momentums and angular momentums in explicit schemes and will be given in the next paper.

References

1. D. Greenspan, *J. Comput. Phys.* **56**, 28 (1984).
2. R. P. Feynman, *The Feynman Lectures on Physics* (Addison–Wesley, Reading, MA, 1963), p. 2.

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