Conservative Numerical Methods for $\ddot{x} = f(x)$

DONALD GREENSPAN

Department of Mathematics, The University of Texas at Arlington,
Arlington, Texas 76019

Received August 11, 1983; revised December 20, 1983

Two distinctly different numerical methods are developed for solving the conservative initial value problem $\ddot{x} = f(x)$, $x(0) = \alpha$, $\dot{x}(0) = \beta$. Both methods conserve exactly the same total energy as does the given differential equation. Computer examples are described and discussed.

1. INTRODUCTION

Physics is characterized by conservation laws and by symmetry [1]. Unfortunately, the application of numerical methodology in approximating solutions of initial value problems usually does *not* preserve either of these invariants. In this sense, the use of a computer destroys the physics of a dynamical model.

We will show here how to conserve total *energy* when solving the nonlinear initial value problem

$$\ddot{x} = f(x); \qquad x(0) = \alpha, \dot{x}(0) = \beta \tag{1.1}$$

on a computer. Moreover, the energy conserved will be exactly that of (1.1), not a new "energy" which is defined by the numerical method (see, e.g., Langdon [6]). Two distinctly different methods will be developed, one of which is completely conservative and symmetric, the other of which reveals how to convert any numerical method to an energy conserving one.

2. PRELIMINARY CONSIDERATIONS

For purposes of intuition and for later convenience in demonstrating structural analogies, let us recall first the proof that (1.1) conserves energy.

Let particle P of *unit* mass be in motion along the X axis. Let the Newtonian dynamical equation of motion and the initial data be given by (1.1). At any time $t = t^*$, let P be located at $x(t^*) = x^*$ and have velocity $\dot{x}(t^*) = v(t^*) = v^*$. Define the work W done by force $f(x)$ during the time $0 \leqslant t \leqslant t^*$ by

$$W = \int_0^{x^*} f(x)\, dx. \tag{2.1}$$

0021-9991/84 $3.00

Then,

$$W=\int_0^{t^*} \tfrac{1}{2}\frac{d}{dt}(\dot{x})^2\,dt=\tfrac{1}{2}(\dot{x}(t^*)]^2-\tfrac{1}{2}[\dot{x}(0)]^2,$$

so that

$$W=K(v^*)-K(\beta), \tag{2.2}$$

where K is kinetic energy. Of course, (2.2) is valid for any $f(x)$.

Now, for a particular $f(x)$, let $\phi(x)$ be any function such that

$$-\frac{d\phi}{dx}=f(x). \tag{2.3}$$

The function $\phi(x)$ is called a potential function for $f(x)$. Then, from (2.1) and (2.3),

$$W=-\phi(x^*)+\phi(a), \tag{2.4}$$

in which ϕ is now called the potential energy.

Elimination of W between (2.2) and (2.4) yields

$$K(v^*)+\phi(x^*)=K(\beta)+\phi(a) \tag{2.5}$$

which is the classical law of conservation of energy.

3. Numerical Method I

The first numerical method is developed from the following observation. Conservation law (2.5) contains $\phi(x)$ explicitly, but not $f(x)$. Thus, if a numerical method is to conserve exactly $K(\beta)+\phi(\alpha)$, the method should incorporate *exactly the same potential function* ϕ as defined in Section 2. Indeed, it need not utilize exactly the same $f(x)$ given in (1.1). With this in mind, we proceed as follows.

For $\Delta t>0$ and $t_k=k\Delta t$, $k=0, 1, 2,\ldots$, let $x(t_k)=x_k$, $v(t_k)=v_k$, $a(t_k)=a_k$. Let $\phi(x)$ satisfy (2.3). Then, assume

$$\frac{v_{k+1}+v_k}{2}=\frac{x_{k+1}-x_k}{\Delta t} \tag{3.1}$$

$$a_k=\frac{v_{k+1}-v_k}{\Delta t}. \tag{3.2}$$

Define $f(x_k) = f_k$ by

$$\begin{aligned} f_k &= -\frac{\phi(x_{k+1}) - \phi(x_k)}{x_{k+1} - x_k}, & x_{k+1} &\neq x_k, \\ &= -\left.\frac{\partial\phi}{\partial x}\right|_{x=x_k}, & x_{k+1} &= x_k, \end{aligned} \tag{3.3}$$

and approximate dynamical equation (1.1) by

$$f_k = ma_k,$$

which, by the assumption of unit mass, reduces to

$$f_k = a_k. \tag{3.4}$$

Let us proceed now as if $x_{k+1} \neq x_k$ in (3.3). Whenever necessary, we will show how to treat the case $x_{k+1} = x_k$. Hence, (3.1)–(3.4) are equivalent to

$$\frac{v_{k+1} + v_k}{2} = \frac{x_{k+1} - x_k}{\Delta t} \tag{3.5}$$

$$\frac{v_{k+1} - v_k}{\Delta t} = -\frac{\phi(x_{k+1}) - \phi(x_k)}{x_{k+1} - x_k}. \tag{3.6}$$

Equations (3.5), (3.6) define x_{k+1}, v_{k+1} implicitly in terms of x_k, v_k. The solution of (3.5), (3.6) for each of $k = 1, 2, \ldots$, from the initial data $x_0 = \alpha$, $v_0 = \beta$, constitutes the numerical solution.

Let us show first that (3.1)–(3.4) conserve exactly the same energy as given in (2.5). In analogy with (2.1), let

$$W_n = \sum_{k=0}^{n-1} (x_{k+1} - x_k) f_k. \tag{3.7}$$

Then

$$\begin{aligned} W_n &= \sum_{k=0}^{n-1} (x_{k+1} - x_k)\, a_k = \sum_{k=0}^{n-1} (x_{k+1} - x_k)\left(\frac{v_{k+1} - v_k}{\Delta t}\right) \\ &= \sum_{k=0}^{n-1} \frac{(x_{k+1} - x_k)}{\Delta t}(v_{k+1} - v_k) = \sum_{k=0}^{n-1}\left(\frac{v_{k+1} + v_k}{2}\right)(v_{k+1} - v_k) \\ &= \tfrac{1}{2}\sum_{k=0}^{n-1} (v_{k+1}^2 - v_k^2) = K(v_n) - K(v_0). \end{aligned}$$

Thus,

$$W_n = K(v_n) - K(\beta), \tag{3.8}$$

in analogy with (2.2).

On the other hand, (3.7) implies

$$\begin{aligned} W_n &= \sum_{k=0}^{n-1} (x_{k+1} - x_k) \left(-\frac{\phi(x_{k+1}) - \phi(x_k)}{x_{k+1} - x_k} \right) \\ &= \sum_{k=0}^{n-1} (-\phi(x_{k+1}) + \phi(x_k)) \\ &= -\phi(x_n) + \phi(x_0), \end{aligned}$$

so that

$$W_n = -\phi(x_n) + \phi(\alpha), \tag{3.9}$$

in complete analogy with (2.4).

Elimination of W_n between (3.8) and (3.9) implies the energy conservation law

$$K(v_n) + \phi(x_n) = K(\beta) + \phi(\alpha), \qquad n = 0, 1, 2, 3, \ldots. \tag{3.10}$$

Since the right sides of (2.5) and (3.10) are identical, it follows that the numerical method conserves exactly the same total energy as does (1.1).

In the case when $x_{k+1} = x_k$, then $\phi(x_{k+1}) - \phi(x_k) = 0$, so that there would be no change in the final summation which led to (3.9). Use of the second formula in (3.3) to calculate W_n would have required the alternative expression

$$-(x_{k+1} - x_k) \left. \frac{\partial \phi}{\partial x} \right|_{x = x_k},$$

which *also* is zero, yielding again no change in the final summation. Thus, conservation law (3.10) is valid in all cases.

Let us show next how to solve (3.5), (3.6) iteratively by means of Newton's method [2]. For fixed k, if (3.5) and (3.6) are rewritten as

$$x_{k+1} = x_k + \frac{\Delta t}{2} (v_{k+1} + v_k) \tag{3.5'}$$

$$v_{k+1} = v_k - (\Delta t) \left(\frac{\phi(x_{k+1}) - \phi(v_k)}{x_{k+1} - x_k} \right), \tag{3.6'}$$

then the Newtonian recursion formulas to be used are

$$x_{k+1}^{(n+1)} = x_k + \frac{\Delta t}{2} (v_{k+1}^{(n)} + v_k) \tag{3.11}$$

$$v_{k+1}^{(n+1)} = v_k - (\Delta t) \frac{\phi(x_{k+1}^{(n+1)}) - \phi(x_k)}{x_{k+1}^{(n+1)} - x_k}, \tag{3.12}$$

with the initial choice $x_{k+1}^{(0)}$, $v_{k+1}^{(0)}$ for the iteration taken to be

$$x_{k+1}^{(0)}=x_k+C_1, \qquad v_{k+1}^{(0)}=v_k+C_2, \tag{3.13}$$

in which C_1, C_2 are constants. If the division by $(x_{k+1}^{(n+1)}-x_k)$ in (3.12) can be, and has been, carried out, then the singularity $x_{k+1}=x_k$ in (3.6′) has been removed, in which case we will always choose $C_1=C_2=0$ in (3.13). This will be illustrated in Example 1. If the division by $(x_{k+1}^{(n+1)}-x_k)$ in (3.12) *cannot* be carried out, but still $x_{k+1}^{(n+1)}\neq x_k$, then one must choose $C_1\neq 0$ in (3.13). This will be illustrated in Example 2.

We now give two examples which not only illustrate the method, but also show clearly that convergence is always to the correct *physical* solution, even when system (3.5), (3.6) has more than one solution.

EXAMPLE 1. Consider the initial value problem

$$\ddot{x}=x^2, \qquad x(0)=1, \dot{x}(0)=1. \tag{3.14}$$

Choosing

$$\phi(x)=-\frac{x^3}{3} \tag{3.15}$$

and noting that

$$E=\frac{1}{2}mv_0^2-\frac{x_0^3}{3}=\frac{1}{2}-\frac{1}{3}=\frac{1}{6}, \tag{3.16}$$

we find that

$$-\frac{\phi(x_{k+1})-\phi(x_k)}{x_{k+1}-x_k}=\frac{1}{3}(x_{k+1}^2+x_{k+1}x_k+x_k^2), \tag{3.17}$$

so that the system to be solved is

$$x_{k+1}=x_k+\frac{\Delta t}{2}(v_{k+1}+v_k) \tag{3.18}$$

$$v_{k+1}=v_k+\frac{\Delta t}{3}(x_{k+1}^2+x_{k+1}x_k+x_k^2). \tag{3.19}$$

The Newtonian iteration formulas, for fixed k, are then

$$x_{k+1}^{(n+1)}=x_k+\frac{\Delta t}{2}(v_{k+1}^{(n)}+v_k) \tag{3.20}$$

$$v_{k+1}^{(n+1)}=v_k+\frac{\Delta t}{3}[(x_{k+1}^{(n+1)})^2+(x_{k+1}^{(n+1)})(x_k)+(x_k)^2] \tag{3.21}$$

$$x_{k+1}^{(0)}=x_k, \qquad v_{k+1}^{(0)}=v_k. \tag{3.22}$$

In applying (3.20)–(3.22), it will be convenient to know, a priori, how many solutions system (3.18), (3.19) has. For this purpose, note that substitution of (3.19) into (3.18), to eliminate v_{k+1}, yields the quadratic equation

$$x_{k+1}^2 + x_{k+1}\left(x_k - \frac{6}{(\Delta t)^2}\right) + \left(x_k^2 + \frac{6}{(\Delta t)^2}x_k + \frac{6}{\Delta t}v_k\right) = 0. \tag{3.23}$$

Since $x_0 = 1$, $v_0 = 1$ are known, let us, for simplicity, consider (3.23) with $k = 0$. An analogous discussion holds for arbitrary k. Hence, $k = 0$, (3.23) reduces to

$$x_1^2 + \left(1 - \frac{6}{(\Delta t)^2}\right)x_1 + \left(1 + \frac{6}{(\Delta t)^2} + \frac{6}{\Delta t}\right) = 0. \tag{3.24}$$

Equation (3.24) has 0, 1, or 2 solutions according as the discriminant $D(\Delta t)$ is less than, equal to, or greater than zero, where

$$D(\Delta t) = \left(1 - \frac{6}{(\Delta t)^2}\right)^2 - 4\left(1 + \frac{6}{(\Delta t)^2} + \frac{6}{\Delta t}\right). \tag{3.25}$$

Since $\lim_{\Delta t \to 0} D(t) = \infty$, there exist two solutions for all sufficiently small Δt. To be precise, let us solve $D(\Delta t) = 0$. This equation is equivalent to the quadratic equation

$$(\Delta t)^4 + 8(\Delta t)^3 + 12(\Delta t)^2 - 12 = 0. \tag{3.26}$$

Equation (3.26) has exactly one real, positive root Δt, and this is the only physically correct solution of (3.26). This solution is

$$\Delta t = -2 + \frac{-\sqrt{8 - \sqrt[3]{256}} + \sqrt{(8 - \sqrt[3]{256}) + 4(8/\sqrt{8 - \sqrt[3]{256}} + (4 + \sqrt[3]{256})/2)}}{2}$$
$$\sim 0.79490525. \tag{3.27}$$

For Δt less than that prescribed by (3.27), Eq. (3.24) has two real roots, and these are given by

$$x_1 = \frac{(6 - (\Delta t)^2) \pm \sqrt{((\Delta t)^2 - 6)^2 - 4(\Delta t)^2((\Delta t)^2 + 6\Delta t + 6)}}{2(\Delta t)^2}. \tag{3.28}$$

If one chooses the positive sign in (3.28), then $\lim_{\Delta t \to 0} x_1 = +\infty$, which is incorrect physically. So, one must choose the negative sign to get the correct root. For $\Delta t = 0.01$, the correct physical approximation, to five decimal places, is

$$x_1 \sim 1.01005, \tag{3.29}$$

while the incorrect solution is $x_1 \sim 59998$.

Table I shows the computer solutions of (3.18), (3.19) by use of (3.20), (3.21) with

TABLE I

x	v	Energy
1.0000000000	1.0000000000	0.166667
1.0100505042	1.0101008418	0.166667
1.0202030372	1.0204057513	0.166667
1.0304596603	1.0309188827	0.166667
1.0408224772	1.0416444964	0.166667
1.0512936345	1.0525869623	0.166667
1.0618753232	1.0637507632	0.166667
1.0725697795	1.0751404983	0.166667
1.0833792864	1.0867608866	0.166667
1.0943061747	1.0986167710	0.166667
1.1053528241	1.1107131220	0.166667
1.1165216650	1.1230550415	0.166667
1.1278151790	1.1356477675	0.166667
1.1392359012	1.1484966777	0.166667
1.1507864211	1.1616072945	0.166667
1.1624693840	1.1749852893	0.166667
1.1742874929	1.1886364874	0.166667
1.1862435097	1.2025668731	0.166667
1.1983402570	1.2167825944	0.166667
1.2105806199	1.2312899687	0.166667
1.2229675471	1.2460954883	0.166667
1.2355040537	1.2612058258	0.166667
1.2481932220	1.2766278403	0.166667
1.2610382042	1.2923685837	0.166667
1.2740422236	1.3084353066	0.166667
1.2872085775	1.3248354652	0.166667
1.3005406384	1.3415767283	0.166667
1.3140418570	1.3586669843	0.166667
1.3277157637	1.3761143484	0.166667
1.3415659713	1.3939271707	0.166667
1.3555961773	1.4121140439	0.166667
1.3698101666	1.4306838116	0.166667
1.3842118136	1.4496455771	0.166667
1.3988050850	1.4690087122	0.166667
1.4135940429	1.4887828666	0.166667
1.4285828471	1.5089779775	0.166667
1.4437757584	1.5296042798	0.166667
1.4591771414	1.5506723163	0.166667
1.4747914677	1.5721929490	0.166667
1.4906233193	1.5941773700	0.166667
1.5066773917	1.6166371137	0.166667
1.5229584976	1.6395840686	0.166667
1.5394715704	1.6630304906	0.166667
1.5562216680	1.6869890160	0.166667
1.5732139764	1.7114726753	0.166667
1.5904538143	1.7364949077	0.166667
1.6079466368	1.7620695763	0.166667
1.6256980396	1.7882109836	0.166667
1.6437137639	1.8149338879	0.166667
1.6619997010	1.8422535203	0.166667
1.6805618966	1.8701856026	0.166667

$\Delta t = 0.01$ up to $k = 50$, which are typical of the more extensive computations carried out. Note that, to ten decimal places,

$$x_1 \sim 1.0100505042, \tag{3.30}$$

which is in complete agreement with (3.29). Indeed, for each k, the computer method converges to the correct physical solution, even though two solutions exist. Note also in Table I that the total energy is always constant and equal to $\frac{1}{6}$ (to the number of decimal places printed).

For the interested reader, the FORTRAN program used is available in Appendix A of Greenspan [3].

EXAMPLE 2. Consider the initial value problem

$$\ddot{x} = -\sin x, \qquad x(0) = \frac{\pi}{2}, \dot{x}(0) = 0, \tag{3.31}$$

for which

$$\phi(x) = -\cos x$$
$$E = \tfrac{1}{2}v_0^2 - \cos x_0 = 0.$$

The system to be solved for each k is

$$x_{k+1} = x_k + \frac{\Delta t}{2}(v_{k+1} + v_k) \tag{3.32}$$

$$v_{k+1} = v_k + (\Delta t)\frac{\cos(x_{k+1}) - \cos x_k}{x_{k+1} - x_k}. \tag{3.33}$$

This time, *unlike* Example 1, the singularity $x_{k+1} = x_k$ in (3.33) is not removable by division. The iteration formulas to be used are, then,

$$x_{k+1}^{(n+1)} = x_k + \frac{\Delta t}{2}(v_{k+1}^{(n)} + v_k) \tag{3.34}$$

$$v_{k+1}^{(n+1)} = v_k + (\Delta t)\frac{\cos(x_{k+1}^{(n+1)}) - \cos x_k}{x_{k+1}^{(n+1)} - x_k} \tag{3.35}$$

$$x_{k+1}^{(0)} = x_k + 1, \qquad v_{k+1}^{(0)} = v_k + 1. \tag{3.36}$$

With $\Delta t = 0.01$, the method converges to the correct physical solution and Table II gives the resulting positions, velocities, and energies through $k = 50$, which are typical of the more extensive calculations which were carried out. Note, again, that the energy is conserved exactly.

TABLE II

x	v	Energy
1.5707963268	0.0000000000	0.000000
1.5707463268	-0.0100000000	0.000000
1.5705963268	-0.0199999999	0.000000
1.5703463268	-0.0299999994	0.000000
1.5699963268	-0.0399999974	0.000000
1.5695463269	-0.0499999920	0.000000
1.5689963270	-0.0599999803	0.000000
1.5683463273	-0.0699999575	0.000000
1.5675963279	-0.0799999174	0.000000
1.5667463291	-0.0899998514	0.000000
1.5657963311	-0.0999997486	0.000000
1.5647463344	-0.1099995955	0.000000
1.5635963395	-0.1199993755	0.000000
1.5623463473	-0.1299990687	0.000000
1.5609963587	-0.1399986516	0.000000
1.5595463750	-0.1499980969	0.000000
1.5579963976	-0.1599973729	0.000000
1.5563464285	-0.1699964436	0.000000
1.5545964700	-0.1799952681	0.000000
1.5527465246	-0.1899938004	0.000000
1.5507965957	-0.1999919892	0.000000
1.5487466868	-0.2099897773	0.000000
1.5465968025	-0.2199871018	0.000000
1.5443469475	-0.2299838932	0.000000
1.5419971276	-0.2399800756	0.000000
1.5395473494	-0.2499755662	0.000000
1.5369976202	-0.2599702750	0.000000
1.5343479483	-0.2699641044	0.000000
1.5315983431	-0.2799569491	0.000000
1.5287488148	-0.2899486958	0.000000
1.5257993752	-0.2999392228	0.000000
1.5227500371	-0.3099283996	0.000000
1.5196008147	-0.3199160868	0.000000
1.5163517236	-0.3299021358	0.000000
1.5130027810	-0.3398863886	0.000000
1.5095540056	-0.3498686769	0.000000
1.5060054181	-0.3598488228	0.000000
1.5023570408	-0.3698266376	0.000000
1.4986088980	-0.3798019221	0.000000
1.4947610161	-0.3897744660	0.000000
1.4908134235	-0.3997440479	0.000000
1.4867661511	-0.4097104346	0.000000
1.4826192320	-0.4196733811	0.000000
1.4783727020	-0.4296326306	0.000000
1.4740265993	-0.4395879134	0.000000
1.4695809649	-0.4495389476	0.000000
1.4650358430	-0.4594854381	0.000000
1.4603912804	-0.4694270766	0.000000
1.4556473274	-0.4793635413	0.000000
1.4508040372	-0.4892944969	0.000000
1.4458614667	-0.4992195939	0.000000

4. Method II

We will show now how to convert any popular numerical method for solving (1.1) so that it is energy conserving. For illustrative purposes, consider a Taylor series method [5], say, for simplicity, of second order,

$$x_{k+1} = x_k + (\Delta t)\, v_k + \frac{(\Delta t)^2}{2} \ddot{x}_k \tag{4.1}$$

$$v_{k+1} = v_k + (\Delta t)\, \ddot{x}_k + \frac{(\Delta t)^2}{2} \dddot{x}_k. \tag{4.2}$$

The error in each of (4.1) and (4.2) is of order $(\Delta t)^3$. We first modify these so that (4.1) has an error of order $(\Delta t)^4$. Thus,

$$x_{k+1} = x_k + (\Delta t)\, v_k + \frac{(\Delta t)^2}{2} \ddot{x}_k + \frac{(\Delta t)^3}{6} \dddot{x}_k \tag{4.3}$$

$$v_{k+1} = v_k + (\Delta t)\, \ddot{x}_k + \frac{(\Delta t)^2}{2} \dddot{x}_k. \tag{4.4}$$

Each final terms in (4.3) and (4.4) now has the *same* derivative of x, that is, $\dddot{x}_k$. Finally, we modify (4.3) and (4.4) by introducing a parameter ε, where

$$\varepsilon = 1 + O(\Delta t), \tag{4.5}$$

in such a fashion that we have

$$x_{k+1} = x_k + (\Delta t)\, v_k + \frac{(\Delta t)^2}{2} \ddot{x}_k + \frac{(\Delta t)^3}{6} \varepsilon \dddot{x}_k \tag{4.6}$$

$$v_{k+1} = v_k + (\Delta t)\, \ddot{x}_k + \frac{(\Delta t)^2}{2} \varepsilon \dddot{x}_k. \tag{4.7}$$

Our problem now reduces to the determination of ε so that E is invariant. Let us show how easily this is done by considering, again, Example 1 of Section 3.

Consider the initial value problem

$$\ddot{x} = x^2, \qquad x(0) = 1,\ \dot{x}(0) = 1. \tag{4.8}$$

For this problem, formulas (4.6) and (4.7) reduce to

$$x_{k+1} = x_k + (\Delta t)\, v_k + \frac{(\Delta t)^2}{2} x_k^2 + \frac{(\Delta t)^3}{3} \varepsilon x_k v_k \tag{4.9}$$

$$v_{k+1} = v_k + (\Delta t)\, x_k^2 + (\Delta t)^2\, \varepsilon x_k v_k. \tag{4.10}$$

We will determine ε so that the change in energy, $\Delta E_k = E_{k+1} - E_k$, is always zero. Thus, since

$$\begin{aligned}\Delta E_k &= E_{k+1} - E_k \\ &= \frac{1}{2}(v_{k+1}^2 - v_k^2) + (\phi(x_{k+1}) - \phi(x_k)) \\ &= \frac{1}{2}(v_{k+1}^2 - v_k^2) + \left(-\frac{x_{k+1}^3}{3} + \frac{x_k^3}{3}\right),\end{aligned}$$

substitution of (4.9) and (4.10) and setting $\Delta E_k = 0$ yields

$$\begin{aligned}&3[(\Delta t)\, x_k^4 + (\Delta t)^3 \varepsilon^2 x_k^2 v_k^2 + 2x_k^2 v_k + 2(\Delta t)\, \varepsilon x_k v_k^2 + 2(\Delta t)^2 \varepsilon x_k^3 v_k] \\ &\quad - 2\left[3x_k^2 \left(v_k + \frac{\Delta t}{2} x_k^2 + \frac{(\Delta t)^2}{3} \varepsilon x_k v_k\right)\right. \\ &\quad + 3x_k \Delta t \left(v_k + \frac{\Delta t}{2} x_k^2 + \frac{(\Delta t)^2}{3} \varepsilon x_k v_k\right)^2 \\ &\quad \left. + (\Delta t)^2 \left(v_k + \frac{(\Delta t)\, x_k^2}{2} + \frac{(\Delta t)^2}{3} \varepsilon x_k v_k\right)^3\right] = 0. \qquad (4.11)\end{aligned}$$

To solve (4.11) iteratively, we define for each k:

$$\varepsilon^{(0)} = 1 \qquad (4.12)$$

$$W = v_k + \frac{\Delta t}{2} x_k^2 + \frac{(\Delta t)^2}{3} \varepsilon^{(n)} x_k v_k \qquad (4.13)$$

$$\begin{aligned}\varepsilon^{(n+1)} &= \{2[W(3x_k^2 + 3x_k W \Delta t + W^2 (\Delta t)^2)] \\ &\quad - 3[x_k^4 \Delta t + (\Delta t)^3 (\varepsilon^{(n)})^2 x_k^2 v_k^2 + 2x_k^2 v_k + 2(\Delta t)^2 \varepsilon^{(n)} x_k^3 v_k]\}/(6x_k v_k^2 \Delta t). \qquad (4.14)\end{aligned}$$

For $\Delta t = 0.01$, Table III shows the resulting values of x_k, v_k, E, and ε through $k = 50$. The results are comparable to those of Table I and each ε is of the form (4.5). For the interested reader, the FORTRAN program used is available in Appendix B of Greenspan [3].

TABLE III

x	v	Energy	Epsilon
1.0000000000	1.0000000000	0.166667	1.000000
1.0100503356	1.0101006714	0.166667	1.006714
1.0202026947	1.0204054019	0.166667	1.006748
1.0304591388	1.0309183454	0.166667	1.006783
1.0408217711	1.0416437619	0.166667	1.006817
1.0512927381	1.0525860210	0.166667	1.006852
1.0618742305	1.0637496050	0.166667	1.006888
1.0725684845	1.0751391127	0.166667	1.006923
1.0833777829	1.0867592628	0.166667	1.006959
1.0943044561	1.0986148978	0.166667	1.006996
1.1053508837	1.1107109875	0.166667	1.007032
1.1165194958	1.1230526338	0.166667	1.007070
1.1278127738	1.1356450737	0.166667	1.007106
1.1392332526	1.1484936847	0.166667	1.007144
1.1507835214	1.1616039886	0.166667	1.007181
1.1624662252	1.1749816563	0.166667	1.007220
1.1742840667	1.1886325126	0.166667	1.007259
1.1862398077	1.2025625411	0.166667	1.007297
1.1983362703	1.2167778893	0.166667	1.007337
1.2105763393	1.2312848740	0.166667	1.007377
1.2229629634	1.2460899866	0.166667	1.007416
1.2354991569	1.2611998992	0.166667	1.007456
1.2481880021	1.2766214702	0.166667	1.007497
1.2610326506	1.2923617504	0.166667	1.007537
1.2740363257	1.3084279900	0.166667	1.007579
1.2872023239	1.3248276443	0.166667	1.007619
1.3005340176	1.3415683811	0.166667	1.007662
1.3140348569	1.3586580881	0.166667	1.007704
1.3277083719	1.3761048796	0.166667	1.007747
1.3415581749	1.3939171045	0.166667	1.007789
1.3555879631	1.4121033547	0.166667	1.007832
1.3698015207	1.4306724725	0.166667	1.007875
1.3842027217	1.4496335603	0.166667	1.007920
1.3987955323	1.4689959888	0.166667	1.007964
1.4135840141	1.4887694062	0.166667	1.008008
1.4285723263	1.5089637488	0.166667	1.008054
1.4437647291	1.5295892498	0.166667	1.008098
1.4591655865	1.5506564509	0.166667	1.008144
1.4747793696	1.5721762127	0.166667	1.008190
1.4906106597	1.5941597255	0.166667	1.008236
1.5066641516	1.6166185224	0.166667	1.008284
1.5229446574	1.6395644901	0.166667	1.008330
1.5394571096	1.6630098830	0.166667	1.008378
1.5562065654	1.6869673352	0.166667	1.008426
1.5731982102	1.7114498757	0.166667	1.008474
1.5904373617	1.7364709414	0.166667	1.008523
1.6079294741	1.7620443936	0.166667	1.008572
1.6256801425	1.7881845327	0.166667	1.008622
1.6436951070	1.8149061145	0.166667	1.008672
1.6619802579	1.8422243678	0.166667	1.008722
1.6805416400	1.8701550119	0.166667	1.008774

5. Remarks

From a scientific point of view, it is of value to apply both Methods I and II to any particular problem, for this would provide the user with a relatively reliable check and balance approach. Individually, Method I is relatively more expensive, since it yields an error in *both* [4] position and velocity of order only $(\Delta t)^3$. However, the conservation property is relatively independent of the convergence tolerance for the Newtonian iteration. Method II can, of course, be adapted to formulas of relatively high accuracy. However, this can be done only with an increasing complexity in the algebraic equation for ε and the conservation property is only accurate to the convergence tolerance used in the iteration.

It is interesting to note also that Method I extends to systems of particles in such a fashion that conservation of energy, and linear and angular momentum can all be conserved exactly as in the continuous case. To do this one need only proceed as follows. For $\Delta t > 0$, let $t_k = k\,\Delta t$, $k = 0, 1, 2, \ldots$, and consider a system of particles P_i, $i = 1, 2, 3, \ldots, n$. Let P_i have mass m_i, and, at time t_k, be located at $\mathbf{r}_{i,k}$ with velocity $\mathbf{v}_{i,k}$ and acceleration $\mathbf{a}_{i,k}$. In analogy with (3.1) and (3.2), assume that

$$\frac{\mathbf{v}_{i,k+1} + \mathbf{v}_{i,k}}{2} = \frac{\mathbf{r}_{i,k+1} - \mathbf{r}_{i,k}}{\Delta t}$$

$$\mathbf{a}_{ik} = \frac{\mathbf{v}_{i,k+1} - \mathbf{v}_{i,k}}{\Delta t}.$$

If $\mathbf{F}_{i,k}$ is the force acting on P_i at time t_k, then force and acceleration are assumed to be related by

$$\mathbf{F}_{i.k} = m_i \mathbf{a}_{i,k}.$$

If $\mathbf{F}_{i,k}$ is a central, $1/r^2$ force, like gravitation or Coulombic interaction, then the arithmetic, conservative force formula is

$$\mathbf{F}_{i,k} = \frac{\alpha(\mathbf{r}_{i,k+1} + \mathbf{r}_{i,k})}{r_{i,k} r_{i,k+1}(r_{i,k} + r_{i,k+1})}.$$

More generally (see, e.g., [4]), if P_i interacts with the other $n - 1$ particles and the force is attractive like $1/r^p$ and repulsive like $1/r^q$, then the arithmetic, conservative force on P_i is given by

$$\mathbf{F}_{i,k} = m_i \sum_{\substack{j=1\\ j \neq i}}^{n} \left[m_j \left(- \frac{G[\sum_{\xi=0}^{p-2} (r_{ij,k}^{\xi} r_{ij,k+1}^{p-\xi-2})]}{r_{ij,k}^{p-1} r_{ij,k+1}^{p-1} (r_{ij,k} + r_{ij,k+1})} + \frac{H[\sum_{\xi=0}^{q-2} (r_{ij,k}^{\xi} r_{ij,k+1}^{q-\xi-2})]}{r_{ij,k}^{q-1} r_{ij,k+1}^{q-1} (r_{ij,k} + r_{ij,k+1})} \right) (\mathbf{r}_{i,k+1} + \mathbf{r}_{i,k} - \mathbf{r}_{j,k+1} - \mathbf{r}_j) \right].$$

Note, however, that the above formulation is both economical and convenient at present only for the case where n is relatively small, such as may be the case in the interaction of large, planetary bodies. Application to plasma simulations, in which $10^3 < n < 10^6$, would be relatively impractical without specially designed computer hardware.

It should be observed also that a number of other papers have been devoted to numerical simulation with exact conservation (see, e.g., [6–8] and the references contained therein). By and large, however, these efforts have been directed toward conserving such quantities as mass, flux, charge, and momentum. Those directed at conservation of energy have not conserved the total energy of the continuous equations being studied.

Finally, let us observe that both theoretical and practical limitations on the choice of Δt which will assure the convergence of Newton's method exist and are at present under study. Though some particular results are known, no general results are available as yet.

References

1. R. P. Feynman, R. B. Leighton, and M. Sands, "The Feynman Lectures on Physics," Addison–Wesley, Reading, Massachusetts, 1963.
2. D. Greenspan, "Discrete Numerical Methods in Pysics and Engineering," Academic Press, New York, 1974.
3. D. Greenspan, Technical Report No. 205, Dept. of Math., Univ. of Texas at Arlington, Arlington, Texas.
4. R. A. LaBudde and D. Greenspan, *Numer. Math.* **25** (1976), 323–346.
5. R. A. LaBudde and D. Greenspan, *Int. J. Math. and Math. Sci.*, in press.
6. A. B. Langdon, *J. Comput. Phys.* **12** (1973), 247–268.
7. Y. P. Popov and A. A. Samarskii, *USSR Comput. Math. Math. Phys.* (*Engl. transl.*) **10** (1970), 265–273.
8. D. Potter, "Computational Physics," Wiley, New York, 1973.