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A note on the equivalence of two recent time-integration schemes for N-body problems

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SUMMARY

This paper investigates the relationship between the energy- and momentum-conserving time-integration scheme of Simo and Gonzalez (*Papers—American Society of Mechanical Engineers—All Series*, 1993; **93**(4)) and a momentum-conserving time-integration scheme due to Betsch and Steinmann (*Int. J. Numer. Meth. Engng* 2000; **49**:599) for N-body problems. The schemes are shown to be identical if the potential energy of interaction between masses is a polynomial function of the distances between the masses, of degree two or lower. In addition, they are shown to recover the same relative equilibria.

KEY WORDS: energy conservation; relative equilibria; time-integration; N-body problem

1. INTRODUCTION

Difficulties arising from the numerical integration of Hamiltonian systems have been prolifically researched in recent years, and a small selection of the results in this area have been given in the list of references, with further sources provided by the references therein. The advantages of using time-integration schemes specifically designed to conserve the first integrals of motion (namely the total energy and momenta for Hamiltonian systems with symmetries) for integrating stiff dynamical systems have been expounded in References [1–7] for problems of non-linear elastodynamics and N-body dynamics. These conservation properties may also be obtained by applying a different technique, using finite elements to discretize the time domain, as shown in References [8, 9].

Important characteristics of the energy- and momentum-conserving algorithms given in References [1–7] are the definition of the algorithmic (nodal) inertial forces as the difference between the (nodal) translational momenta (at the beginning and end of the current time-step) divided by the time-step length, and an appropriate definition of the algorithmic (nodal) potential forces which satisfies the conservation requirements. For example, the energy–momentum algorithm of Simo and Tarnow (developed for non-linear elastodynamics of

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St. Venant–Kirchhoff materials [3]) uses the average of the Second Piola–Kirchhoff stresses at the beginning and end of the observed time-step: note that these are *not* the stresses computed at the average positions. Taking the stresses computed at the average positions results in the symplectic mid-point scheme given in Reference [4]. This scheme, however, is not energy-conserving, and has been widely reported as unsuitable for stiff dynamical systems [1–3, 5, 7].

Betsch and Steinmann [8] have recently proposed another (closely related) interpretation of the nodal potential forces in the context of N-body problems. They suggest defining the algorithmic force of interaction between two masses as the force computed at the average *distance* between the two masses over the considered time-step, and demonstrate its surprisingly good performance numerically. In this short note, we show that the method of Betsch and Steinmann is in fact energy-conserving if the potential energy of interaction between masses is a particular type of polynomial function of the distances between the masses.

2. OUTLINE OF ALGORITHMS

The energy- and momentum-conserving algorithm proposed independently by Greenspan [6, 10] for $N=1$ and 3 and Simo and Gonzalez [1] for general N can be written as

$$\mathbf{r}^i_{n+1} - \mathbf{r}^i_n - \frac{\Delta t}{2m^i}(\mathbf{p}^i_{n+1} + \mathbf{p}^i_n) = \mathbf{0} \tag{1}$$

$$\mathbf{p}^i_{n+1} - \mathbf{p}^i_n - \Delta t \sum_{\substack{j=1,\\ j\neq i}}^{N} \frac{V(l^{ij}_{n+1}) - V(l^{ij}_n)}{(l^{ij}_{n+1})^2 - (l^{ij}_n)^2}(\mathbf{r}^{ij}_{n+1} + \mathbf{r}^{ij}_n) = \mathbf{0} \tag{2}$$

for bodies $i=1,\ldots,N$ where $\mathbf{r}^i_n$, $\mathbf{p}^i_n$ and m^i denote the position and linear momentum vectors and the mass, respectively, of body i at time-step n, and $V(\cdot)$ represents the potential energy of interaction between masses, which we refer to as the potential function. The time-step length is given by Δt. For brevity, we write $\mathbf{r}^{ij}_n = \mathbf{r}^j_n - \mathbf{r}^i_n$, and thus $l^{ij}_n = \|\mathbf{r}^{ij}_n\| \equiv \sqrt{\mathbf{r}^{ij}_n \cdot \mathbf{r}^{ij}_n}$ is the distance between bodies i and j at time-step n. We will refer to this algorithm as Algorithm 1.

The momentum-conserving algorithm of Betsch and Steinmann [8] (named the *Assumed Distance Method* by the authors) can be written as

$$\mathbf{r}^i_{n+1} - \mathbf{r}^i_n - \frac{\Delta t}{2m^i}(\mathbf{p}^i_{n+1} + \mathbf{p}^i_n) = \mathbf{0} \tag{3}$$

$$\mathbf{p}^i_{n+1} - \mathbf{p}^i_n - \Delta t \sum_{\substack{j=1,\\ j\neq i}}^{N} \frac{V'(l^{ij}_{n+1/2})}{l^{ij}_{n+1} + l^{ij}_n}(\mathbf{r}^{ij}_{n+1} + \mathbf{r}^{ij}_n) = \mathbf{0} \tag{4}$$

where $V'(x)$ represents the derivative of the potential function with respect to x. We will refer to this algorithm as Algorithm 2.

3. COMPARISON OF ALGORITHMS

Algorithm 2 is not energy-conserving in general, but was reported to perform surprisingly well when tested on the numerical examples given in Reference [8]. A clue to this unexpectedly good performance may lie in the similarity of Algorithm 2 to Algorithm 1, which is known to be energy-conserving: upon examination, we see that Equations (1) and (3) are identical, and Equations (2) and (4) differ only in the scalar term inside the summation sign; namely $[V(l_{n+1}^{ij}) - V(l_n^{ij})]/[(l_{n+1}^{ij})^2 - (l_n^{ij})^2]$ in Algorithm 1 and $V'(l_{n+1/2}^{ij})/(l_{n+1}^{ij} + l_n^{ij})$ in Algorithm 2.

Proposition
For potential functions that are polynomials of degree two or lower, Algorithms 1 and 2 are identical.

Starting with the term $[V(l_{n+1}^{ij}) - V(l_n^{ij})]/[(l_{n+1}^{ij})^2 - (l_n^{ij})^2]$ in Algorithm 1 and treating l_n^{ij} as a fixed value, we can express $V(l_{n+1}^{ij})$ as a Taylor series expansion about the point l_n^{ij}, i.e. $V(l_{n+1}^{ij}) \equiv V[l_n^{ij} + (l_{n+1}^{ij} - l_n^{ij})] = \sum_{s=0}^{\infty} V^{(s)}(l_n^{ij})/s!(l_{n+1}^{ij} - l_n^{ij})^s$. Thus we have

$$\frac{V(l_{n+1}^{ij}) - V(l_n^{ij})}{(l_{n+1}^{ij})^2 - (l_n^{ij})^2} = \frac{1}{l_{n+1}^{ij} + l_n^{ij}} \sum_{s=0}^{\infty} \frac{V^{(s+1)}(l_n^{ij})}{(s+1)!} (l_{n+1}^{ij} - l_n^{ij})^s \tag{5}$$

Similarly, with the term $V'(l_{n+1/2}^{ij})/(l_{n+1}^{ij} + l_n^{ij})$ in Algorithm 2, we can write $V'(l_{n+1/2}^{ij}) \equiv V'[l_n^{ij} + \frac{1}{2}(l_{n+1}^{ij} - l_n^{ij})] = \sum_{s=0}^{\infty} V^{(s+1)}(l_n^{ij})/(2^s s!)(l_{n+1}^{ij} - l_n^{ij})^s$. Now we have

$$\frac{V'(l_{n+1/2}^{ij})}{l_{n+1}^{ij} + l_n^{ij}} = \frac{1}{l_{n+1}^{ij} + l_n^{ij}} \sum_{s=0}^{\infty} \frac{V^{(s+1)}(l_n^{ij})}{2^s s!} (l_{n+1}^{ij} - l_n^{ij})^s \tag{6}$$

Comparing (5) with (6) reveals that the first and second terms of each series are identical, given that $(s+1)! = 2^s s!$ for $s = 0, 1$. Thus for potential functions $V(\cdot)$ such that $V^{(s+1)}$ vanishes for $s \geqslant 2$, Equations (5) and (6), and thus Algorithms 1 and 2, are identical: this class of functions is precisely the set of polynomials of degree two or lower.

Corollary
For potential functions that are polynomials of degree two or lower, Algorithm 2 is energy-conserving.

Comparing (5) with (6) also reveals that Algorithms 1 and 2 are identical in the case where $l_{n+1}^{ij} = l_n^{ij}$ $\forall i, j, n$ since then only the first term in each series expansion is non-zero. This condition holds for relative equilibrium motions of the system, e.g. uniformly translating or rotating motions where the forces of interaction match the inertial and applied forces for each body, and so the bodies move in unison while their relative positions with respect to one another remain constant. Hence Algorithm 2 recovers the same relative equilibria as Algorithm 1. The latter correspond, up to a relative group motion, to the relative equilibria of the underlying physical system, regardless of the time-step length [11], which is a desirable property not present in many popular time-integration schemes.

Of course, in general we have $l_{n+1}^{ij} \neq l_n^{ij}$ for at least some i, j, n. However, for problems where the forces of interaction *approximately* match the inertial and applied forces, the change in length is small, and thus $l_{n+1}^{ij} \approx l_n^{ij}$ $\forall i, j, n$. In this case, the powers $(l_{n+1}^{ij} - l_n^{ij})^s$ in each series

decay rapidly to zero as s increases, and thus the algorithms produce very similar results: hence for these problems, Algorithm 2 will be 'almost' energy-conserving, which may help to explain its impressive performance.

For a practical example of a potential function where Algorithms 1 and 2 may coincide, consider the strain energy potential for linear materials, which can be written as

$$V(l_n^{ij}) \equiv \phi(l_n^{ij}) = \tfrac{1}{2}k[\varepsilon(l_n^{ij})]^2(\bar{l}^{ij})^2 \tag{7}$$

where $\varepsilon(\cdot)$ is a strain measure to be defined. Here, k is the stiffness constant and $\bar{l}^{ij}$ denotes the original distance between the two bodies, such that $V'(\bar{l}^{ij}) = V(\bar{l}^{ij}) = 0$, where $V'(\cdot)$ represents the magnitude of the force of interaction between the bodies. For the algorithms to coincide, $V(l_n^{ij})$ must not contain powers of l_n^{ij} higher than $(l_n^{ij})^2$, which means that $\varepsilon(l_n^{ij})$ can be at most linear in l_n^{ij}. Now consider two popular strain measures; the (*Rotated*) *Engineering strain*

$$\varepsilon(l_n^{ij}) = \frac{l_n^{ij}}{\bar{l}^{ij}} - 1 \tag{8}$$

and *Green's strain*

$$\varepsilon(l_n^{ij}) = \frac{1}{2}\left(\frac{(l_n^{ij})^2}{(\bar{l}^{ij})^2} - 1\right) \tag{9}$$

(see Reference [12] for details). We immediately see that the use of the Engineering strain in conjunction with the strain energy potential (7) fulfils the condition for Algorithm 2 to be energy-conserving. However, the use of Green's strain with the strain energy potential (7) (thus giving the St. Venant–Kirchhoff material model), often lauded for the simplicity of the mathematical expressions it produces, does not fulfil this condition.

4. NUMERICAL EXAMPLE

For completeness, we include a numerical demonstration of the energy conservation properties of Algorithm 2 when applied to problems with the strain energy potential (7) using Engineering strain. Our model problem is the spring–mass system (Figure 1) as given by Simo *et al.* in Reference [4]; thus the potential function for this problem is

$$V(l_n^{ij}) = \frac{1}{2}k\left(\frac{l_n^{ij}}{\bar{l}^{ij}} - 1\right)^2(\bar{l}^{ij})^2 = \frac{1}{2}k(l_n^{ij} - \bar{l}^{ij})^2$$

and the material parameters are $k=1.0$, $m^i=1.0$ and $\bar{l}^{ij}=1.0\ \forall i,j$. The initial position and linear momentum vectors $\mathbf{r}_0^i$ and $\mathbf{p}_0^i$, generated randomly by the authors, are

$$\mathbf{r}_0^1 = \langle 0.2340, -0.2166, -0.0109\rangle^{\mathrm{T}}, \qquad \mathbf{p}_0^1 = \langle 0.04095, -0.01483, 0.04325\rangle^{\mathrm{T}}$$

$$\mathbf{r}_0^2 = \langle 0.0772, 0.7605, 0.0061\rangle^{\mathrm{T}}, \qquad \mathbf{p}_0^2 = \langle -0.02980, 0.04400, -0.02959\rangle^{\mathrm{T}}$$

$$\mathbf{r}_0^3 = \langle 0.8054, 0.6466, -0.1059\rangle^{\mathrm{T}}, \qquad \mathbf{p}_0^3 = \langle -0.02328, -0.01432, -0.03716\rangle^{\mathrm{T}}$$

$$\mathbf{r}_0^4 = \langle 0.3903, 0.6187, 0.9678\rangle^{\mathrm{T}} \quad \text{and} \quad \mathbf{p}_0^4 = \langle 0.04152, 0.00114, 0.02621\rangle^{\mathrm{T}}$$

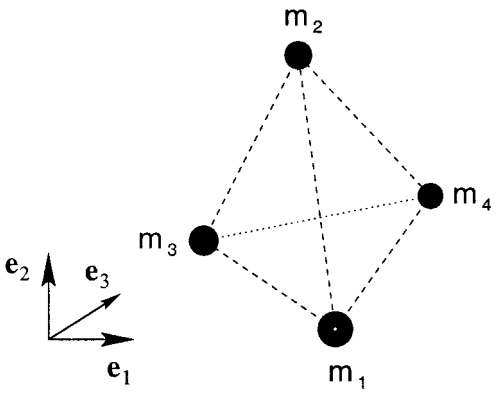

Figure 1. Spring–mass system [5].

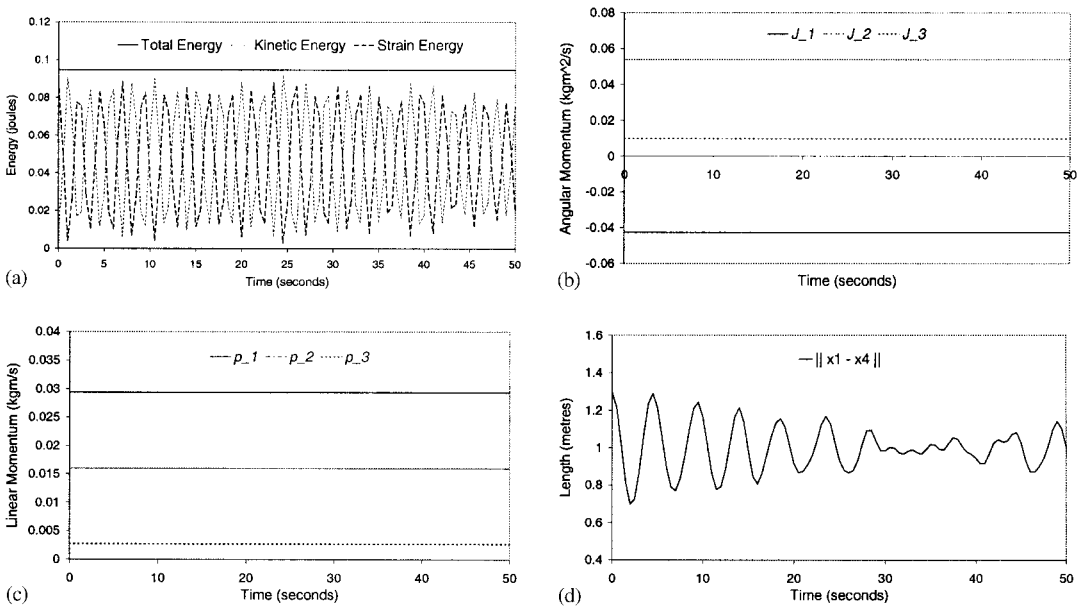

Figure 2. Performance of Algorithm 2 for $\Delta t = 0.5$: (a) energy; (b) angular momentum; (c) linear momentum; and (d) length between two masses.

Note that the reference positions $\bar{\mathbf{r}}^i$ (which ensure that $V(\bar{l}^{ij}) = 0\ \forall i, j$) and initial displacements $\mathbf{r}_0^i - \bar{\mathbf{r}}^i$ of each body are therefore indeterminate (although the initial lengths l_0^{ij} are fully defined): in fact they are arbitrary, provided the resulting initial position vectors $\mathbf{r}_0^i$ are as given above. Figure 2 shows the energy and momentum conservation of Algorithm 2 when applied to this problem using a time-step size of $\Delta t = 0.5\ \forall n$. Graphs (a)–(c) can readily be compared with those in Figure 9 of Reference [5], obtained using an energy–momentum algorithm

called the *projection method* by the authors, which has since been superseded in terms of performance by Algorithm 1. Graph (d) can be visually compared to the corresponding graph in Figure 8 of Reference [4], although the time-step used there is $\Delta t = 0.01$.

5. CONCLUSIONS

An interesting relationship between two recent momentum-conserving time-integration schemes has been shown. By applying a Taylor series expansion, the newly proposed momentum-conserving algorithm for N-body problems due to Betsch and Steinmann [8] has been shown to be energy-conserving provided the potential energy of interaction between masses is a polynomial function of the distances between the masses, of degree two or lower, whereupon it is identical to the energy–momentum algorithm of Simo and Gonzalez [1]. The same argument has shown that the two algorithms recover the same relative equilibria, which are known to be those of the underlying physical system, up to a group motion. Consequently, for a general potential function, the two algorithms are shown to give very similar results provided that the distances between pairs of masses remain more or less constant: in this case, the algorithm of Betsch and Steinmann can be said to be 'almost' energy-conserving.

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