Journal of Sound and Vibration (2002) **252**(5), 935–944
doi:10.1006/jsvi.2001.4044 available online at http://www.idealibrary.com on IDEAL®

SOME REMARKS ON THE NUMERICAL TIME INTEGRATION OF NON-LINEAR DYNAMICAL SYSTEMS

P. B. Bornemann, U. Galvanetto and M. A. Crisfield

Imperial College of Science, Technology and Medicine, Prince Consort Road, London SW7 2BY, England. E-mail: u.galvonetto@ic.ac.uk

(*Received* 9 *July* 2001, *and in final form* 2 *October* 2001)

1. INTRODUCTION

During the last two decades the study of small non-linear dynamical systems has known a tremendous growth. The complexity and richness of their dynamics have captured the attention of the researchers who are increasingly using numerical algorithms to explore dynamics that can only be partially investigated with analytical tools. Some potential pitfalls of the numerical integration have been highlighted in several papers, see for example reference [1], but it is often believed that an accurate time integration scheme with small time steps can deal with most non-linear dynamical systems. One of the most widely used time integration algorithms is the family of the explicit Runge–Kutta schemes, especially the fourth order members, see for example references [2–5] and a practically infinite number of other papers. These methods are very general, easy to implement and fourth order accurate. In discrete linear systems, where a finite number of natural frequencies can be detected, it is sometimes assumed that a time step equal to a small fraction of the smallest natural period is sufficient to guarantee the accuracy of the integration, where small fraction means equal to 1/50-1/30 [6]. Moreover, very often only the steady state behaviour is investigated and therefore the initial transient is disregarded, but in this way one could lose some information interesting from a numerical point of view, as explained later. In the case of conservative problems it is often believed that a small time step is sufficient to prevent numerical instabilities, i.e., to maintain the total energy of the system close to its exact value. In this paper, it is shown how a small error in the total energy does not necessarily corresponds to a small error in the solution.

In structural engineering implicit time integration schemes are commonly used to investigate the long-term dynamics of systems in which high frequencies are not present or can be neglected. One of the most popular implicit schemes is Newmark's method [7] that is general and, for the parameter choice of the present work, unconditionally stable for linear problems. However, this stability is not maintained for non-linear problems and hence a range of energy–momentum conserving schemes have been proposed [8, 9] for mechanical systems. Both, Newmark's method and energy–momentum methods are at most second order accurate. It will be shown how these lower order implicit time integration methods achieve a better solution in a conservative mechanical problem, the rigid circular pendulum, in particular if energy conservation is guaranteed. The main drawback of the energy conserving methods is their lack of generality since different energy conserving schemes have to be developed for different systems of differential equations.

0022-460X/02/$35.00

The paper is organized as follows: section 2 presents the problem of a simple pendulum. Two explicit fourth order Runge–Kutta schemes and three second order implicit schemes are described in section 3. Finally, in section 4, the results of these numerical integrators of section 3 to a long-time integration of the pendulum of section 2 are compared to the exact solution given in the same section.

2. SIMPLE RIGID PENDULUM

Figure 1 shows the system under investigation: a 1-d.o.f. rigid pendulum. The angle, θ, between the pendulum and the vertical direction, is the only degree of freedom of the system, while ℓ is the constant length and m indicates a point mass at the tip of the truss. The gravity field is defined in the negative y direction by the constant acceleration g. No additional external or damping forces are applied.

The motion of the pendulum is described by the non-linear second order differential equation

$$m\ell\ddot{\theta} + mg\sin\theta = 0, \qquad \theta(t_0) = \theta_0, \qquad \dot{\theta}(t_0) = \dot{\theta}_0 \tag{1}$$

with initial conditions θ_0 and $\dot{\theta}_0$. The system is conservative therefore the total energy (or Hamiltonian) H, sum of kinetic energy K and potential energy V are constant as shown by the following equations:

$$\begin{aligned} H = K + V &= \tfrac{1}{2}m\ell^2\dot{\theta}^2 - mg\ell\cos\theta = H_0, \\ H_0 &= \tfrac{1}{2}m\ell^2\dot{\theta}_0^2 - mg\ell\cos\theta_0. \end{aligned} \tag{2}$$

An analytical solution of the motion is given in reference [10, Chapter 1].

$$\theta(t) = 2\arcsin\left(k\cdot\mathrm{sn}(t\sqrt{g/\ell},k)\right), \quad k = \sqrt{\frac{1}{2}\left(1 + \frac{H}{mg\ell}\right)}. \tag{3}$$

Equation (3) contains the Jacobian elliptic function sn and its modulus k.

3. TIME INTEGRATION SCHEMES

Numerical time integration is performed for $t_0 \leqslant t \leqslant t_N$ at discrete time steps $t_{n+1} = t_n + \Delta t_n, n = 0, \ldots, N$, with time step size $\Delta t_n > 0$. The numerical approximations of angle and angular velocity at t_n are $\theta_n \approx \theta(t_n)$ and $\dot{\theta}_n \approx \dot{\theta}(t_n)$.

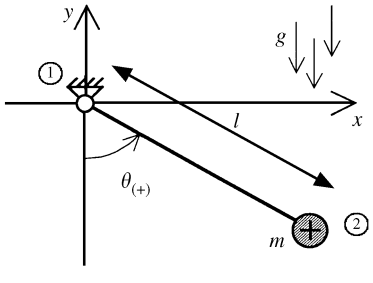

Figure 1. 1-d.o.f. pendulum.

3.1. RUNGE–KUTTA METHODS

The widely used fourth order accurate Runge–Kutta methods, Kutta4 and Fehl-berg4, e.g., references [2, 11, 12], are used to integrate equation (1). Since these explicit schemes are first order integrators, equation (1) has to be transformed into a system of two first order ODEs, where $\mathrm{p}^{\mathrm{T}} = [p_1\, p_2] = [\theta\, \dot{\theta}]$:

$$\dot{p}(t) = \begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \end{bmatrix} = \begin{bmatrix} \dot{\theta} \\ \ddot{\theta} \end{bmatrix} = \begin{bmatrix} \dot{\theta} \\ -\frac{g}{\ell}\cos\theta \end{bmatrix} = \begin{bmatrix} p_2 \\ -\frac{g}{\ell}\cos p_1 \end{bmatrix} = \mathbf{F}(t, \mathbf{p}(t)). \tag{4}$$

The general definition of a Runge–Kutta scheme with s-stages is given by

$$\mathbf{k_i} = \mathbf{F}(t_n + c_i \Delta t_n, \mathbf{p}_n + \Delta t_n \sum_{j=1}^{s} a_{ij}\mathbf{k}_j), \quad i = 1, \ldots, s,$$

$$\mathbf{p}_{n+1} = \mathbf{p}_n + \Delta t_n \sum\nolimits_{j=1}^{s} b_j \mathbf{k}_j, \tag{5}$$

where the constant parameters c_i, a_{ij} and b_j $(i,j = 1, \ldots, s)$ are different for each Runge–Kutta scheme. Equation (6) displays these parameter for Kutta4 ($s=4$) in the convenient Butcher scheme, where the column corresponds to c_i and the row to b_j. The main diagonal and upper triangle of matrix a_{ij} are zero which is necessary for explicit schemes. Similarly, Butcher's scheme for five-stages Fehlberg4 is expressed in equation (7). Additionally, the fifth order companion, Fehlberg5 ($s=6$), is introduced. This embedded scheme will be later used for an adaptive time-stepping algorithm [11, 12].

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline p^{K4}_{n=1} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \tag{6}$$

$$\begin{array}{c|ccccc} 0 & & & & & \\ \frac{1}{4} & \frac{1}{4} & & & & \\ \frac{3}{8} & \frac{3}{32} & \frac{9}{32} & & & \\ \frac{12}{13} & \frac{1932}{2197} & \frac{7296}{2197} & 0 & & \\ 1 & \frac{439}{216} & -8 & \frac{3680}{513} & -\frac{845}{4104} & \\ \hline \frac{1}{2} & -\frac{8}{27} & 2 & -\frac{3544}{2565} & \frac{1859}{4104} & -\frac{11}{40} \\ \hline P^{Fb4}_{n+1} & \frac{25}{216} & 0 & \frac{1408}{2565} & \frac{2197}{4104} & -\frac{1}{5} \\ \hline P^{Fb5}_{n+1} & \frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & -\frac{9}{50} \quad \frac{2}{55} \end{array} \tag{7}$$

3.2. NEWMARK'S METHOD

Newmark's method [7] is based on a linear interpolation of acceleration with two control parameters $0 \leqslant \gamma \leqslant 1$ *and* $0 \leqslant \beta \leqslant \frac{1}{2}$. In *linear* structural dynamics the choice $\gamma \geqslant \frac{1}{2}, \beta \geqslant \frac{1}{4}(\gamma + \frac{1}{2})^2$ [13] guarantees unconditional stability for any time step size $\Delta t_n > 0$ (A-stability).

For the rigid pendulum, Newmark's method is given as

$$\frac{\theta_{n+1} - \theta_n}{\Delta t_n} = \dot{\theta}_n - \frac{\Delta t_n}{2}\Big((1 - 2\beta)\frac{g}{\ell}\sin\theta_n + 2\beta\frac{g}{\ell}\sin\theta_{n+1}\Big), \tag{8}$$

$$\frac{\dot{\theta}_{n+1} - \dot{\theta}_n}{\Delta t_n} = -(1 - \gamma)\frac{g}{\ell}\sin\theta_n - \gamma\frac{g}{\ell}\sin\theta_{n+1}. \tag{9}$$

In the remainder the parameters are fixed with $\gamma = \frac{1}{2}$, $\beta = \frac{1}{4}$. This scheme is referred to as average acceleration method or trapezoidal rule (TR) and is an implicit, second order accurate Runge–Kutta method. Although it preserves the energy in linear Hamiltonian mechanical systems, this property is not retained in conservative non-linear dynamical systems.

3.3. ENERGY–MOMENTUM METHOD

Originally, Simo *et al.* [8] designed energy–momentum methods which take advantage of the fact that certain properties, such as total energy, translational and angular momenta, are conserved in some dynamical systems. Energy–momentum methods preserve these properties independent of the time step size, see references [8, 9, 14].

The energy–momentum method (EMM) needs two different parts, angular velocity and angular acceleration, to discretize the second order differential equation of pendulum (1).

$$\frac{\theta_{n+1} - \theta_n}{\Delta t_n} = \frac{\dot{\theta}_{n+1} - \dot{\theta}_n}{2}, \tag{10}$$

$$\frac{\dot{\theta}_{n+1} - \dot{\theta}_n}{\Delta t_n} = \frac{1}{m\ell}\frac{V(\theta_n) - V(\theta_{n+1})}{\ell(\theta_{n+1} - \theta_n)} = -\frac{g}{\ell}\frac{\cos\theta_n - \cos\theta_{n+1}}{\theta_{n+1} - \theta_n}. \tag{11}$$

The potential energy $V(\theta) = -mg\ell\cos\theta$, as in equation (2), is used to express equation (11) which is an algorithmic version of equation (1) designed to conserve the total energy (2). Obviously, this part differs for different mechanical systems. The presented formulae (11) and (10), the latter basically the trapezoidal rule, are second order accurate.

The conservation of total energy can be demonstrated by computing the change of energy between time t_n and t_{n+1}. Equations (10, 11) are introduced in equation (2):

$$\begin{aligned}\frac{H_{n+1} - H_n}{\Delta t_n} &= \frac{m\ell^2}{2\Delta t}\Big(\dot{\theta}_{n+1}^2 - \dot{\theta}_n^2\Big) + \frac{mg\ell}{\Delta t_n}(\cos\theta_n - \cos\theta_{n+1}) \\ &= m\ell^2\left[-\frac{g}{\ell}\frac{\cos\theta_n - \cos\theta_{n+1}}{\theta_{n+1} - \theta_n}\right]\left[\frac{\theta_{n+1} - \theta_n}{\Delta t_n}\right] + mg\ell\frac{\cos\theta_n - \cos\theta_{n+1}}{\Delta t_n} = 0.\end{aligned} \tag{12}$$

Similarly, preservation of angular momentum for $g = 0$ can be shown. However, all presented time integration schemes conserve angular momentum in this special case of the 1-d.o.f. pendulum without gravity ($g = 0$), because the mechanical system is described in equation (1) by the liner differential equation $\ddot{\theta} = 0$ and the appropriate initial conditions.

3.4. "SINE-BASED" MIDPOINT METHOD

As an alternative to the energy–momentum method of section 3.3, a "sine-based" midpoint method (SIM), which also conserves total energy is constructed. Again, discrete versions for the angular velocity and for the angular acceleration form the time integration rule as follows:

$$\frac{2\sin(\Delta\theta/2)}{\Delta t_n} = \frac{\dot\theta_{n+1} + \dot\theta_n}{2} \quad \text{and} \quad \Delta\theta = \theta_{n+1} - \theta_n, \tag{13}$$

$$\frac{\dot\theta_{n+1} - \dot\theta_n}{\Delta t_n} = -\frac{g}{\ell}\sin\theta_{n+1/2} \quad \text{with } \theta_{n+1/2} = \frac{\theta_{n+1} + \theta_n}{2}. \tag{14}$$

An examination of the local discretization error of equations (13) and (14) shows that the "sine-based" midpoint method is second order accurate. The same idea as in equation (12) can be applied to demonstrate the property of energy conservation for an arbitrarily large time step size.

4. EXAMPLE

In the example problem Figure 2 with truss length $\ell = 1$ m and point mass $m = 1$ kg, the initial position was chosen at $\theta_0 = -\pi$ with a small angular velocity $\dot\theta_0 = 10^{-3}\ \mathrm{s}^{-1}$. The pendulum rotates continuously anticlockwise due to the initial angular velocity under the effect of gravity $g = 9{\cdot}8\ \mathrm{m/s^2}$ with a constant total energy of $H_0 = \frac{1}{2}m\ell^2\dot\theta_0^2 - mg\ell\cos\theta_0 = 9{\cdot}800\,0005$ N m.

At first, the pendulum equation was integrated from $t_0 = 0$ s to $t_N = 50\,000$ s with a fixed time step size $\Delta t = 0{\cdot}01$ s. The period can be determined with $T \approx 6{\cdot}470\,7897$ s, so the step size corresponds to roughly 650 steps per period. The results of the different time integration schemes are shown in Figure 3. Although all implicit schemes, trapezoidal rule (TR), energy–momentum method (EMM) and "sine-based" midpoint method (SIM) are close to the analytical solution, both explicit schemes depart from the reference.

However, the course of total energy, as shown in Figure 4 in the form of relative deviation $\Delta\bar H = (H_n - H_0)/H_0$, exhibits smaller energy errors for the explicit schemes compared to the trapezoidal rule. At the end of the integration Fehlberg4 deviates by $\approx 0{\cdot}001\%$, Kutta4 by $\approx -0{\cdot}002\%$, whereas TR by $\approx -0{\cdot}03\%$.

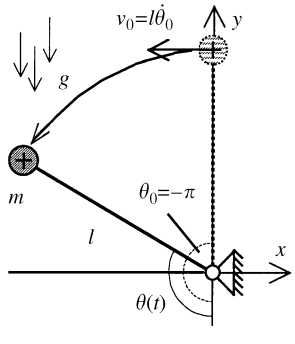

Figure 2. Initial configuration of example.

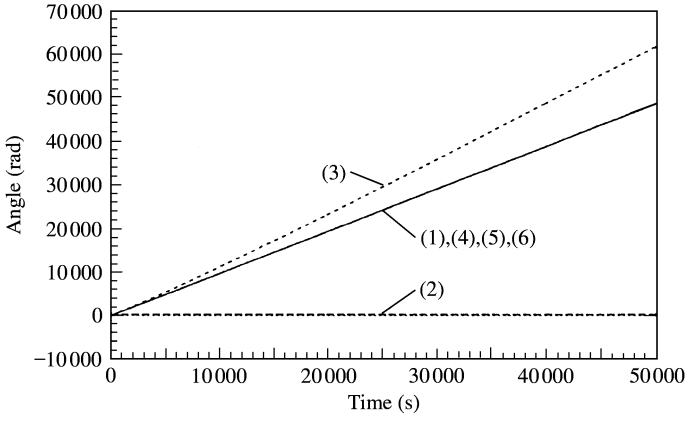

Figure 3. Angle versus time, fixed time step size $\Delta t = 0 \cdot 01$ s : ——, (1): Reference; ------, (2): Kutta4;-----, (3): Fehlberg4; ....., (4): TR; -·-·-·-·-, (5): EMM; -··-··-··-, (6) SIM.

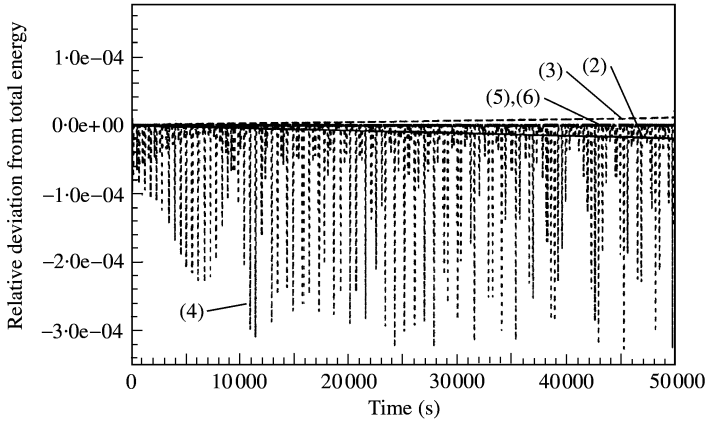

Figure 4. Total energy versus time, fixed time step size $\Delta t = 0 \cdot 01$ s : ——, (2): Kutta4; ----, (3): Fehlberg4; -----, (4): TR;....., (5): EMM; -··-··-··-, (6) SIM.

The energy-conserving schemes react as expected and no energy-fluctuations are observable.

In Figures 5 and 6, the initial time histories of angle and total energy over a shorter time are magnified. The solution of the Fehlberg4 algorithm rotates increasingly quickly as the energy level rises, whereas the numerical energy consumption of the Kutta4 scheme leads to a qualitative change of the result at $t \approx 190$ s. At this time, the total energy falls below the critical energy level of $H_{\dot{\theta}=0,\, T=\infty} = 9{\cdot}8$ N m, which represents a state with no initial velocity, see also reference [10]. The pendulum oscillates rather than rotating in the following integration.

The application of the adaptive time integration scheme Fehlberg4 (5) [12] improves the result, see Figure 7. However, with an absolute tolerance limit of $tol = 10^{-10}$ the number of integration steps was almost doubled $N = 9\,402\,523$ leading to an average step size of $\Delta t_{average} \approx 5{\cdot}317 \times 10^{-3}$ s. The step size minimum was $\Delta t_{min} \approx 2{\cdot}221 \times 10^{-3}$ s and the

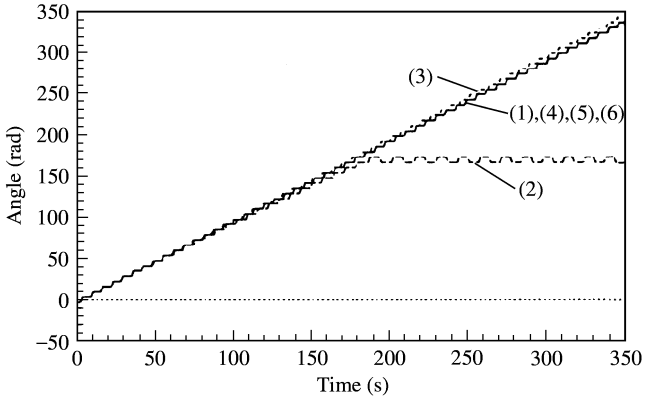

Figure 5. Angle versus time, fixed time step size $\Delta t = 0 \cdot 01$ s : ——, (1): Reference; - - - - - -, (2): Kutta4;- - - - -, (3): Fehlberg4; ....., (4): TR; - · - · - · - ·, (5): EMM; - · - · - · - ·, (6) SIM.

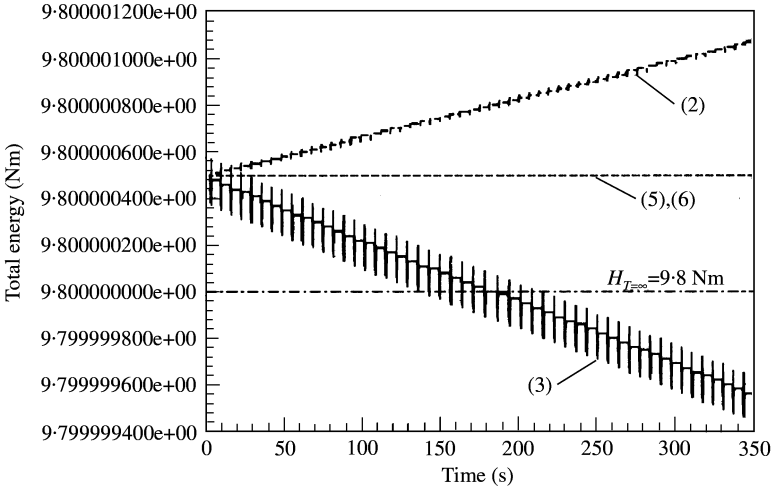

Figure 6. Total energy versus time, fixed time step size $\Delta t = 0 \cdot 01$ s : ——, (2): Kutta4; - - - - - -, (3): Fehlberg4; - - - - -, (5): EMM; ....., (6) SIM.

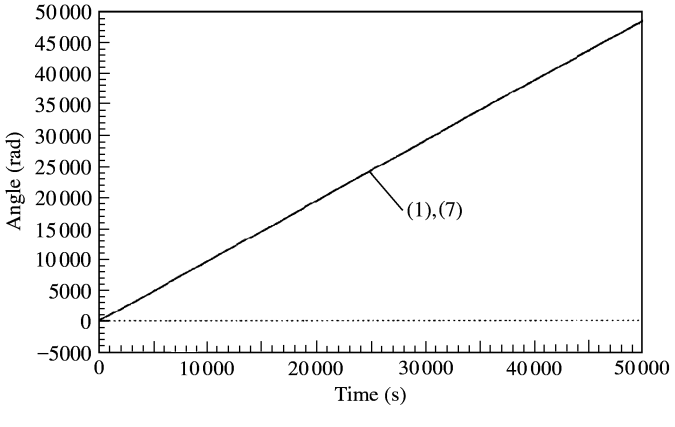

Figure 7. Adaptive algorithm Fehlberg4 (5): Angle versus time ——, (1): Reference; - - - - - -, (7): Fehlberg4 (5).

maximum $\Delta t_{max} \approx 5{\cdot}524 \times 10^{-3}$ s. In Figure 8, the deviation of total energy is compared to the *numerical* divergence for the energy-conserving methods.

Finally, the problem under investigation was solved with a larger time step, $\Delta t = 0{\cdot}15$ s corresponding to 43 points per period. For the chosen integration interval $0\text{ s} \leqslant t \leqslant 50\,00\,0\text{ s}$ $N = 333\,333$ steps are used. Figures 9 and 10 show how Kutta 4 switches again to a low-energy level oscillation, Fehlberg4 finds a fast spinning solution at a high-energy level, TR does not diverge but finds a solution with no physical meaning, whereas EMM and SIM still find reasonable solutions. The results obtained by the trapezoidal rule seems to contradict its property of A-stability, but the concept of A-stability only holds for the integration of linear differential equations. Figure 11 shows the total energy computed by the three implicit integration methods: with the larger time step, the energy computed by TR can be affected by an error larger than 7%.

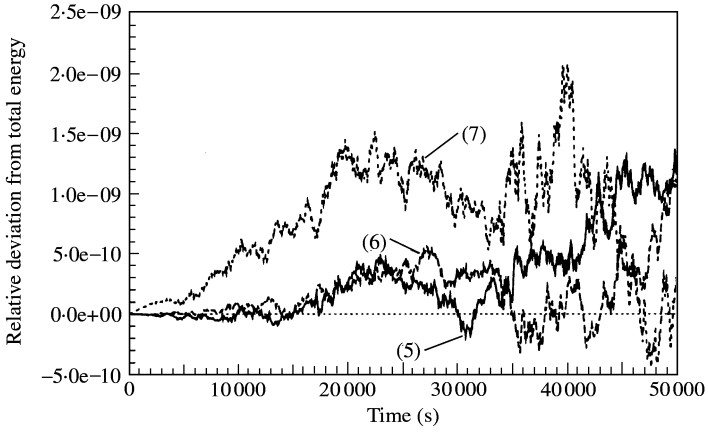

Figure 8. Relative deviation from total energy $(H(t) - H_0)/H_0$ versus time ——, (5):EMM $\Delta t = 0{\cdot}01$ s ; ------, (6): SIM $\Delta t = 0{\cdot}01$ s; ------, (7): Fehlberg4(5).

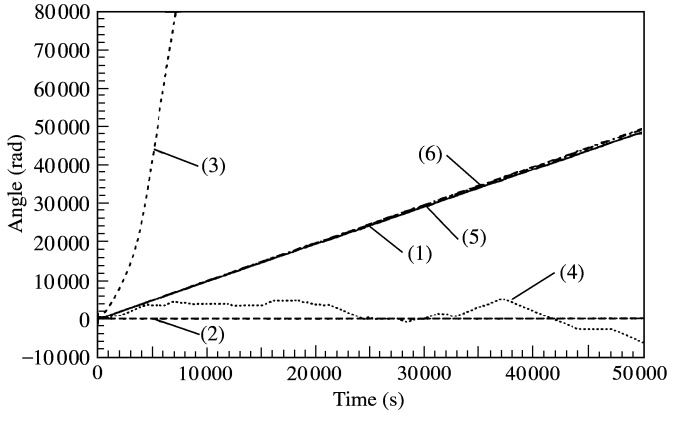

Figure 9. Angle versus time, fixed time step size $\Delta t = 0{\cdot}15$ s : ——, (1): Reference; - - - -, (2): Kutta4;------, (3): Fehlberg4; . . . . ., (4): TR;- · - · - ·, (5): EMM; - · - · - · - ·, (6) SIM.

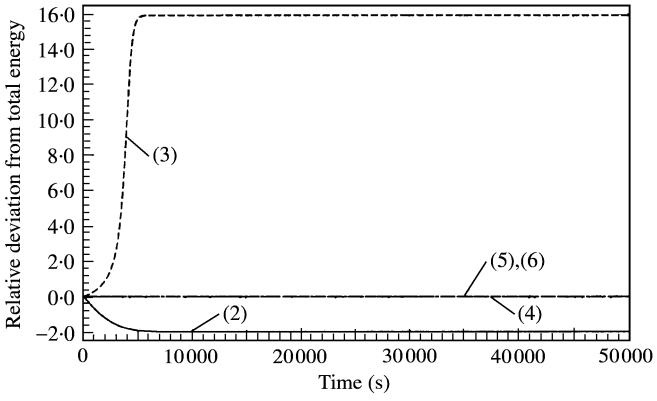

Figure 10. Relative deviation from total energy $(H(t) - H_0)/H_0$ versus time, fixed time step size $\Delta t = 0{\cdot}15$ s : —— (2): Kutta4;- - - - -, (3): Fehlberg4; - - - - -, (4): TR; ....., (5): EMM; - · - · - · - ·, (6) SIM.

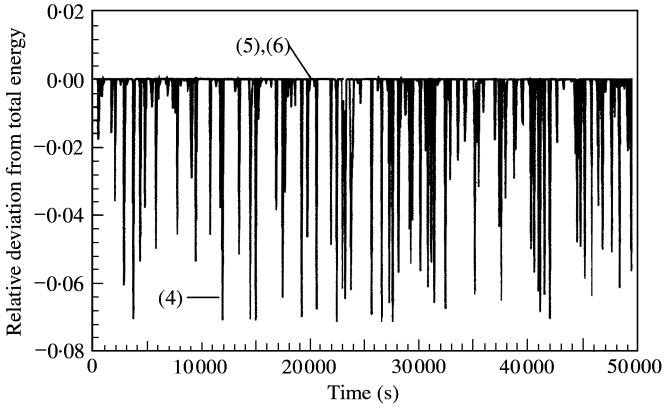

Figure 11. Implicit schemes: relative deviation from total energy $(H(t) - H_0)/H_0$ versus time, fixed time step size $\Delta t = 0{\cdot}15$ s : ——,(4): TR; - - - - - -, (5): EMM;- - - - - -, (6) SIM.

5. CONCLUSIONS

A conservative, non-linear dynamic problem has been numerically integrated with different algorithms and the relevant solutions have been compared to the exact reference solution. Initially, a small time step has been chosen (650 time steps per period). The higher order schemes, Kutta4 and Fehlberg4, provide the worst solution. On the contrary, all the implicit methods, that are only second order accurate, calculate a much more accurate solution. Surprisingly, the energy computed by Kutta4 and Fehlberg4 is practically constant during the integration whereas the energy computed by TR is affected by a greater error; therefore, monitoring the total energy of the system during the numerical integration would not necessarily provide a reliable check on the accuracy of the solution. For a larger time step, the conserving schemes still provide a reasonable answer whereas TR converges to a meaningless solution. Hence, it seems that the property of energy conservation has a considerable influence on the quality of the solution for this conservative mechanical problem. Indeed, for more complex problems for which the

potential includes the strain energy, it has been found that both energy and momentum conservation can be important [8, 9, 14]. For a hypothetical dissipative system the results might be different. Nonetheless, even for dissipative systems it would seem sensible to introduce algorithms that retain the conservation properties in the limit as the dissipation tends to zero.

The main conclusion of the present work is that caution must be used when integrating even simple non-linear systems with popular fourth order Runge–Kutta explicit algorithms. Numerical solutions so obtained should always be compared with other solutions obtained with other algorithms, possibly derived from energy–momentum conserving schemes.

ACKNOWLEDGMENTS

Support for the presented work was provided by EPSRC under GR/N05673. This support is gratefully acknowledged.

REFERENCES

1. P. G. Reinhall, T. K. Caughey and D. W. Storti 1989 *American Society of Mechanical Engineers Journal of Applied Mechanics* **56**, 162–166. Order and chaos in a discrete duffing oscillator: implications on numerical integration.
2. R. Seydel 1988 *From Equilibrium to Chaos, Practical Bifurcation and Stability Analysis*. New York: Elsevier.
3. U. Galvanetto and S. R. Bishop 1998 *Computer Methods in Applied Mechanical Engineering* **163**, 373–382. Computational techniques for nonlinear dynamics in multiple friction oscillators.
4. B. L. Van de vrande, D. H. Van Campen and A. De Kraker 1999 *Nonlinear dynamics* **19**, 157–169. An approximate analysis of dry-friction-induced stick–slip vibrations by a smoothing procedure.
5. B. H. K. Lee, S. J. Price and Y. S. Wong 1999 *Progress in Aerospace Sciences* **35**, 205–334. Nonlinear aeroelastic analysis of airfoils: bifurcation and chaos.
6. J. Nussbaum and A. Ruina 1987 *Pure and Applied Geophysics* **125**, 629–656. A 2 degree-of-freedom earthquake model with static/dynamic friction.
7. N. M. Newmark 1959 *Journal of the Engineering Mechanic Division* **85**, 67–94. A method of computation for structural dynamics.
8. J. C. Simo, N. Tarnow and K. K. Wong 1992 *Computer Methods in Applied Mechanical Engineering* **100**, 63–116. Exact energy-momentum conserving algorithms and symplectic schemes for nonlinear dynamics.
9. M. A. Crisfield and J. Shi 1994 *International Journal for Numerical Methods in Engineering* **37**, 1897–1913. A co-rotational element/time integration strategy for non-linear dynamics.
10. M. Tabor 1989 *Chaos and Integrability in Nonlinear Dynamics*. New York: John Wiley & Sons.
11. E. Hairer, S. P. Nørsett and G. Wanner 1987 *Solving Ordinary Differential Equations I, Nonstiff Problems*. Berlin: Springer-Verlag.
12. R. L. Burden and J. D. Faires 1988 *Numerical Analysis*. Boston: PWS-Kent; fourth edition.
13. E. Ramm 1997 *Stabtragwerke Teil* VII, *Baudynamik*. Stuttgart: Institut für Baustatik, Universität Stuttgart.
14. O. Gonzalez 1996 *Journal of Nonlinear Science* **8**, 449–467. Time integration and discrete Hamiltonian systems.