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BUILDING A BETTER LEAPFROG

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ABSTRACT

In stellar dynamical computer simulations, as well as other types of simulations using particles, time step size is often held constant in order to guarantee a high degree of energy conservation. In many applications, allowing the time step size to change in time can offer a great saving in computational cost, but variable-size time steps usually imply a substantial degradation in energy conservation. We present a "meta-algorithm" for choosing time steps in such a way as to guarantee time symmetry in any integration scheme, thus allowing vastly improved energy conservation for orbital calculations with variable time steps. We apply the algorithm to the familiar leapfrog scheme, and generalize to higher order integration schemes, showing how the stability properties of the fixed-step leapfrog scheme can be extended to higher order, variable-step integrators such as the Hermite method. We illustrate the remarkable properties of these time-symmetric integrators for the case of a highly eccentric elliptical Kepler orbit and discuss applications to more complex problems.

Subject headings: celestial mechanics, stellar dynamics — galaxies: star clusters

1. INTRODUCTION

Time-symmetry is a desirable property of an integration scheme because of its inherent energy conservation properties. The simplest such scheme, known as the leapfrog or Verlet method (Hockney & Eastwood 1988), gained extra popularity when it was shown to be also the simplest example of the class of symplectic schemes (Channel & Scovel 1990; Yoshida 1990; Sanz-Serna & Calvo 1994). However, the time-symmetry of an integrator is spoiled when the integration time step length is allowed to vary during the calculation—indeed, Skeel & Gear (1992) have shown that any integration scheme which is symplectic for constant time step cannot retain its symplectic character when the time step is changed in explicit dependence on *instantaneous* position and velocity. In this *Letter*, we report on a practical means of circumventing this problem and describe the construction of a very general class of time-symmetric integration algorithms with both arbitrarily variable time steps and excellent energy conservation. As a specific example, we present a simple fourth-order generalization of the leapfrog scheme and show how the improvements due to time symmetrization carry over to this case.

The leapfrog integration scheme is a standard way of integrating the equations of motion of interacting particles whose interactions have no explicit velocity dependence. Examples of such simulations are found in stellar dynamics, in plasma physics, and in molecular dynamics (where the leapfrog scheme is more commonly known as the Verlet method) (Hockney & Eastwood 1988; Barnes & Hut 1986). Usually, the leapfrog is written in a time-interleaved way, in which positions and velocities are specified at alternating points in time, as follows:

$$r_1 = r_0 + v_{1/2}\,\delta t\,, \tag{1a}$$

$$v_{3/2} = v_{1/2} + a_1\,\delta t\,, \tag{1b}$$

where r can stand for the position vector of a single particle or the combined vector $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N$ representing a system of N particles. The quantity $v = dr/dt$ is the velocity and $a(t) = a[r(t)] = dv/dt$ is the acceleration. The subscripts after the various quantities indicate the time at which they apply, in units of the time step, i.e., $v_{1/2} = v(t + \frac{1}{2}\,\delta t)$. One reason for the popularity of this integration scheme is its simplicity and ease of coding. Another is its often surprisingly high accuracy and stability compared with other second-order schemes (e.g., Runge-Kutta methods). Note that the displacement of v with respect to r and a is time symmetric, preventing any systematic build-up of energy error in time.

For many applications the typical accuracy attainable by a leapfrog scheme is not high enough. Specifically, the presence of a large range in length and time scales may make the use of constant step size impractical (Hut, Makino, & McMillan 1988; Makino & Hut 1988, 1990). In this *Letter* we present two ways of generalizing the leapfrog scheme to deal with more demanding applications, while preserving its main desirable properties. First, we show how the time step length can be varied from step to step; second we offer a version with fourth-order accuracy (the leapfrog described by eq. [1] is only second-order accurate). We then demonstrate the usefulness of these symmetrized schemes to the integration of particle orbits in the N-body problem.

2. THE LEAPFROG SCHEME WITH VARIABLE TIME STEPS

It is convenient to map the standard interleaved description into a form in which all variables are defined at the same instant in time:

$$r_1 = r_0 + v_0\,\delta t + \tfrac{1}{2}a_0(\delta t)^2\,, \tag{2a}$$

$$b_1 = v_0 + \tfrac{1}{2}(a_0 + a_1)\delta t\,. \tag{2b}$$

Starting from $\{r_0, v_0, a_0\}$, one first computes r_1, then a_1 (r_1), by evaluating the appropriate expression dictated by the system under consideration, and finally v_1. The velocity equation can alternatively be written as a predictor step:

$$v_{1p} = v_0 + a_0\,\delta t\,, \tag{3a}$$

followed by a corrector step:

$$v_{1c} = v_{1p} + \tfrac{1}{2}(a_1 - a_0)\delta t\,. \tag{3b}$$

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The position step is a pure predictor one and has no need for a corrector so long as we require only second-order accuracy. While equation (2) looks as though it has lost its explicit time symmetry, it is still equivalent to the original equation (1), as can be verified by direct substitution (Barnes & Hut 1989; Tuckerman, Berne, & Martyna 1992).

From equation (2), the first generalization to time-dependent time step sizes would seem trivial. At each new point in time, one can choose an appropriate value of δt depending on the requirements of the physical system being modeled (smaller time steps during close approaches of two or more particles, say). However, this strategy can easily fail miserably, not only in the case of the leapfrog (Skeel 1993) but equally in the case of higher order symplectic integration schemes (Calvo & Sanz-Serna 1993). The main problem is the fact that step size variability destroys the explicit time symmetry of the leapfrog.

Our alternative approach does not affect the force calculations themselves, but instead is based on a prescription for recovering time symmetry. The central idea is to change the time step in such a way as to guarantee time symmetry to the level of accuracy required, using an implicit time step criterion and iteration to reach convergence. Note, however, that iteration, although convenient, is not an essential part of our approach. If the necessary force evaluation were prohibitively expensive, one could maintain a list of several previous time step sizes, and use polynomial extrapolation to predict the next time step in advance.

The implicit form of our time-symmetrized integration scheme can be written in the leapfrog case as follows:

$$\xi_1 = f(\xi_0, \delta t)\,, \tag{4a}$$

$$\delta t = \tfrac{1}{2}[h(\xi_0) + h(\xi_1)]\,, \tag{4b}$$

where $\xi = (r, v)$ is the $2N$-dimensional phase space vector for a system with N degrees of freedom, and the function f is defined through equation (2). Note that the presence of the a_1 term at the right-hand side of equation for v_1 in equation (2) does not introduce a ξ_1 dependence in the equation for ξ_1 above, since in equation (2) a_1 may be obtained directly as a function of r_0 and v_0 through its functional form $a_1[r_1(r_0, v_0)]$. We solve these implicit equations iteratively and simultaneously for all particles in the system. There are many possible choices for the time step criterion h. We have chosen one of the simplest: the minimum overall particle pairs of the interparticle encounter and free-fall times.

Figure 1 shows the result of an integration of the Kepler two-body problem for an elliptical orbit with eccentricity $e = 0.9$ for 10 orbital periods with 10^3 integration steps per orbit. The motion is fully described by the four orbital elements: eccentricity e, semimajor axis a, time of pericenter passage T_p, and longitude of pericenter l. These four quantities are plotted as osculating elements in Figure 1. Note the near-constancy of a, apart from the nearly periodic errors, and the linear drift in T_p (as opposed to the quadratic growth of phase error typical of most integration schemes).

The same behavior is plotted for an integration over 10^3 orbits in Figure 2. The horizontal line in Figure 2 (*top*) shows the results of our iterated solution (the first and higher iterations are indistinguishable on this scale). The naive variable-time leapfrog (*diagonal line*) can be seen to fail badly, growing to an error of nearly 1% after 1000 orbits. By comparison, our algorithm gives a final error $\Delta a/a < 10^{-6}$ after 10^3 orbits, even in the case of only one iteration per step. The maximum error

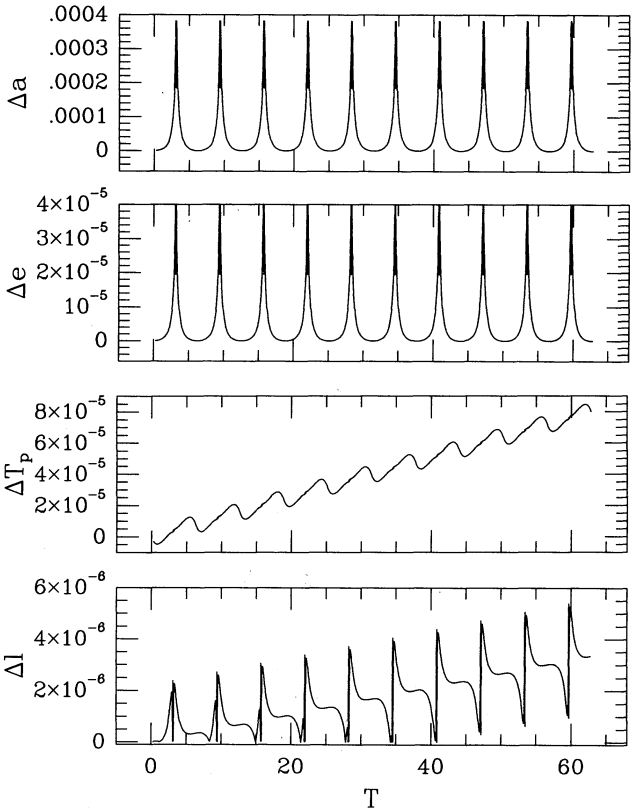

FIG. 1.—Variable–time step time-symmetric leapfrog integration (eq. [2]) of an elliptic Kepler orbit with eccentricity 0.9, for 10 orbital periods (20π time units). Only one iteration step is used to provide an explicit approximation to our implicit definition of a time-symmetric choice of time steps (eq. [4]). The four panels show the variation of the four osculating orbital elements of this two-dimensional problem: (*top*) semimajor axis a; (*second*) eccentricity e; (*third*) time of pericenter passage T_p; (*bottom*) longitude of pericenter l. There is no significant drift in a (or in energy $E \propto 1/a$), even though the per orbit energy errors are significant near pericenter. The phase error remains constant per orbit, resulting in the linear growth evident in the third panel.

per orbit remains at the level visible in Figure 1 (*top*), $\Delta a/a \lesssim 4 \times 10^{-4}$. Thus, the long time buildup, even for 1000 orbits, would be invisible on the vertical scale used in Figure 1 (*top*). In the second and third panels of Figure 2, the curves for the time of pericenter passage T_p show, at different scales, how a second iteration per time step can further improve accuracy in this particular application. A constant–time step leapfrog integration gives significantly worse errors than the naive variable–time step scheme during a single orbit (a factor 20 larger than the vertical scale of Fig. 2 [*top*], for the same number of steps per orbit), although its time-symmetric properties still prevent the linear growth of energy error shown by the latter scheme.

On the face of it, these results seem to conflict with the theoretical analysis of Skeel & Gear (1992; see also Calvo & Sanz-Serna 1993) showing that variable step size seriously degrades the performance of symplectic integration schemes. However, since Skeel & Gear considered only explicit time step criteria based on information available at the beginning of a time step, their approach precludes a time symmetrization of the type proposed here.

3. FOURTH-ORDER GENERALIZATION

In simulations with a large range of length and time scales, second-order integration schemes are often not sufficient, even

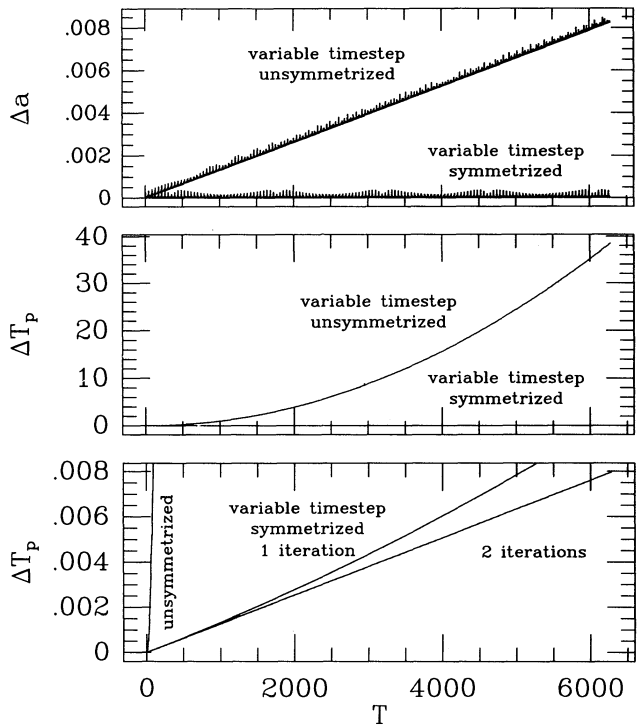

FIG. 2.—The same Kepler ellipse integration as in the previous figure, extended to cover the first 10^3 orbits. *Top*: The long-term stability of the energy is reflected in the stability of the semimajor axis a. The horizontal curve is the extension of Fig. 1 (*top*) for a hundredfold longer time period. For comparison, the diagonally slanted curve shows the result of applying the leapfrog algorithm (eq. [2]) straightforwardly to a time-variable time step scheme *without* time symmetrization (the uneven "fray" above the lines is due purely to limited sampling frequency). *Middle*: The time of pericenter passage T_p. Note the quadratic build-up of phase error for the non–time-symmetric scheme, as opposed to the near-constancy of T_p for our iterative implementation of a time-symmetric scheme. *Bottom*: The same as the middle panel on a larger vertical scale. The nonsymmetric scheme is now represented as a near-vertical line. The diagonal line is the result of taking two corrector steps per time step, while the intermediate line gives the result of single iteration.

with our time-symmetrized improvements. Fortunately, our approach carries over smoothly and straightforwardly to higher order. We first applied our iterative time-symmetrization to the Hermite algorithm (Makino 1991; Makino & Aarseth 1992), the state-of-the-art integration scheme used in simulations of dense star systems.

The following truncated form of the Hermite scheme (a type of Obrechkoff method [Lambert 1973, e.g., p. 201, eq. [4]) clearly brings out the fact that it is the natural generalization of the leapfrog:

$$r_1 = r_0 + \tfrac{1}{2}(v_1 + v_0)\delta t - \tfrac{1}{12}(a_1 - a_0)(\delta t)^2 , \qquad (5a)$$

$$v_1 = v_0 + \tfrac{1}{2}(a_1 + a_0)\delta t - \tfrac{1}{12}(j_1 - j_0)(\delta t)^2 , \qquad (5b)$$

where the jerk $j = da/dt$ is calculated directly by differentiation of the expression for the force (thereby introducing a dependency on velocity as well as position in the case of Newtonian gravitational forces). In this fourth-order scheme, equation (4a) may be rewritten as

$$\xi_1 = g(\xi_0, \xi_1, \delta t) , \qquad (6)$$

where the function g is defined by equation (5).

Figure 3 illustrates the remarkable properties of the symmetrized Hermite scheme in the integration of a Kepler ellipse with $e = 0.999$. As in the second-order scheme, 10^3 steps were used per orbit integration. For comparison, we have used a second-order scheme for this nearly linear orbit in the standard nonsymmetrized leapfrog way and found a disastrous error build-up of more than 100%. Applying a single iteration per step, this error was reduced to a drift of $\Delta a/a \simeq 5 \times 10^{-5}$, but with spikes of $\Delta a/a \simeq 0.05$. After two iterations, convergence was reached to a level of $\Delta a/a \simeq 10^{-7}$, and no further improvement could be reached for 10^3 steps per orbit. For Hermite, a single iteration resulted in a drift of $\Delta a/a \simeq 10^{-6}$, while two iterations per step gave $\Delta a/a \simeq 2 \times 10^{-10}$. Three or more iterations quickly converged to a residual drift of $\Delta a/a \simeq 10^{-10}$. We have applied the scheme to more eccentric orbits, finding similar stability properties even in the extreme case $e = 0.999{,}999$.

4. DISCUSSION

The enormous improvement in long-term stabilbity of the time-symmetric integration schemes shown here is partly due to the strictly periodic nature of a Kepler orbit. However, the advantages of our approach are not limited to periodic applications. Figure 4 shows a representative set of results for

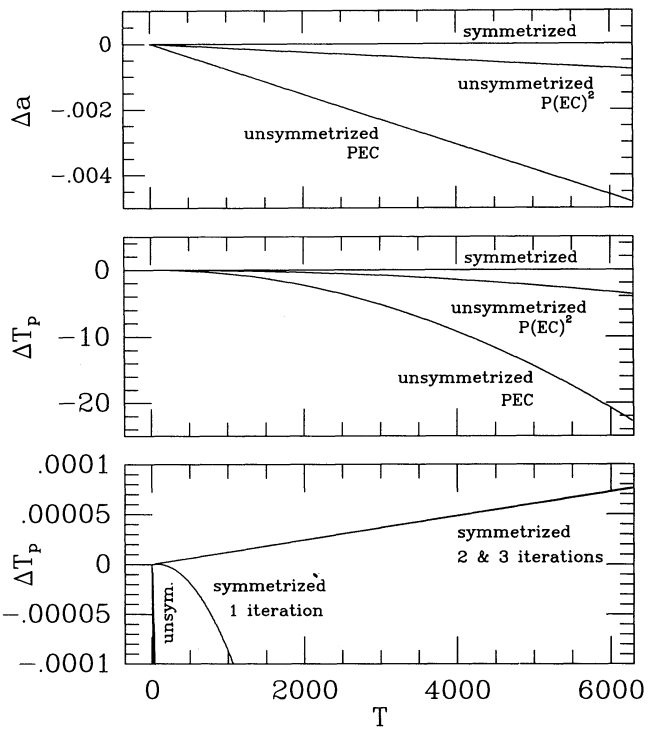

FIG. 3.—A fourth-order generalized-leapfrog integration (eq. [5]) of a Kepler ellipse with eccentricity $e = 0.999$. *Top*: The lowest, diagonal line shows the linear drift in energy (and thereby semimajor axis) for the standard PEC (Predict Evaluate Correct) Hermite integration scheme used in stellar dynamics of star cluster simulations [14, 15]. The middle line shows how an additional (Evaluate Correct) force calculation at the end of each time step gives a modest improvement, but not enough to offset the extra cost (since we could alternatively halve the time step and thereby improve the accuracy by a factor ~ 16). The top line shows the result of using a once-iterated symmetric time step implementation, leading to an improvement of a factor $\gg 16$. *Middle*: These three lines correspond to the three schemes used in the top panel. *Bottom*: An enlargement in the vertical direction of the middle panel, where now the lowest two curves nearly coincide into one thick almost-vertical line. The intermediate curve here is the result of a once-iterated symmetric time step. The far more accurate line extending toward the right gives the result of two iterations per time step. For our choice of overall time step size, leading to 10^3 steps per orbit, further iteration provides little extra benefit.

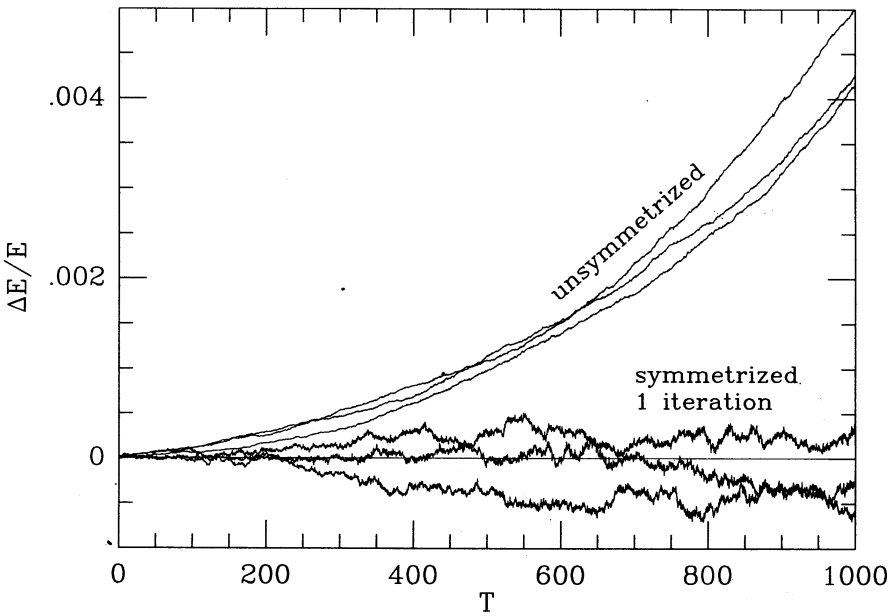

FIG. 4.—Six independent 100 body runs, starting from Plummer-model initial conditions, each taking roughly the same amount of computer time. The top three lines show the growth of the relative energy error in each run as a function of time for the standard unsymmetrized variable-time step leapfrog scheme. The bottom three lines show the same data for the symmetrized version of the code.

several 100 body systems integrated with exactly the same leapfrog codes as were used in Figure 2, with a variable time step size, shared by all particles. The greatly improved accuracy of the symmetrized scheme (as well as the nonsystematic nature of its energy error) is clearly evident. Time steps were chosen such that each run took roughly the same amount of computer time, so the actual step sizes are twice as large in the time-symmetric (one-iteration) runs than in the unsymmetrized cases.

In all cases studied so far, we have found substantial improvements, leading us to be optimistic that general N-body integrations, in gravitational as well as other particle simulation problems, will gain significantly from time-symmetrization. A discussion of these simulations, including the extension of the method to include individual (Aarseth 1985) and block (McMillan 1986) time steps, is beyond the scope of the present *Letter* and will be reported elsewhere. However, it is worth pointing out that had we included a substantial fraction of initial binary systems, such as are found in most (if not all) real star clusters, the unsymmetrized integrator would have inherited all of the errors presented in Figures 2 and 3 and fared even worse in comparison to the symmetrized scheme.

To illustrate the stability of our algorithm, we have integrated the well-known Pythagorean problem (Szebehely & Peters 1967, hereafter SP), a complex three-body problem with many close encounters. With three iterations per time step, and with comparably many force evaluations as in SP, we reversed the velocities at time $t = 62$ (the value used by SP) and ran our integration back to $t = 0$, reproducing the initial positions with errors in the third decimal place; a reversal at $t = 32$ gave an error in the ninth place. These results compare well with those obtained by SP, despite the fact that our scheme, unlike theirs, includes no regularization of close encounters (for a regularized extension of our method, see Funato et al. 1995). The errors are quite consistent with the expected degradation in accuracy due to the amplification of double-precision (64 bit) round-off errors by close encounters, indicating that the time-reversibility test is satisfied to as high a degree of accuracy as can be expected.

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