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Abstract

A smooth time-step selection formula for the midpoint method is derived which minimize deviations in the Hamiltonian function along piecewise-linear phase space trajectories of autonomous Hamiltonian systems. The time-step formula is implemented in a second order predictor/corrector scheme and applied to Kepler's problem. The formula significantly improves energy conservation as well as the accuracy of the configuration space trajectory. Peak errors in position and momentum coordinates are not significantly reduced, but the time behavior of the errors is markedly more regular.

Key Words: energy conserving methods, implicit methods, midpoint method, discrete mechanics, variational principles, principle of least action, Hamiltonian differential equations

Mathematics Subject Classifications: 65L12, 70H05

1 Introduction

Hamiltonian dynamical systems arise naturally in classical mechanics, geometric optics, optimal control theory and a wide variety of other situations in which the basic phenomena of interest can be characterized by a variational principle [4]. Considerable interest exists in developing computational algorithms which exploit the special properties of Hamiltonian dynamics.

Conservation of energy (or more generally, conservation of the Hamiltonian function) is one of the basic properties of Hamiltonian dynamics. In this paper, we show how this property is exploited in a new variable time-step midpoint scheme for Hamiltonian systems. Time-step sizes are chosen to minimize the deviations in the Hamiltonian function along a piecewise-linear, continuous interpolation of the discrete trajectory determined by the midpoint scheme. The new variable-step midpoint scheme is implemented in a simple predictor/corrector algorithm and comparisons are made with a fixed-step implementation of the same predictor/corrector algorithm. The total number of function evaluations are kept the same for both variable-step and fixed-step schemes. Simulation results show that for Kepler's problem, the variable-step scheme produces markedly better orbits than does the fixed-step scheme. This is achieved with the small overhead of the one vector/matrix multiplication and the one vector/vector dot product used to determine the size of each time-step.

The ideas contained in this paper originated from the author's work on a discrete-time theory for Hamiltonian dynamics called DTH dynamics [10, 11, 12]. DTH dynamics determines piecewise-linear, continuous, phase space trajectories which exactly conserve the Hamiltonian function at the midpoints of each linear segment. In the extended phase space formulation of Hamiltonian dynamics (where time is treated like a position coordinate) the principle of least action does not uniquely determine how time behaves. Using a discrete version of the principle of least action, T. D. Lee [5] showed that for Newtonian potential systems, the behavior of time is governed by the conservation of energy. Using a new discrete variational principle, the author has shown that the behavior of time in DTH dynamics is governed by conservation of the Hamiltonian function. Existence and uniqueness results as well as asymptotic results characterizing the behavior of time in DTH dynamics are given in [10]. We use a different approach here. Instead of attempting to exactly conserve the Hamiltonian function, we instead minimize deviations

in the value of the Hamiltonian along the entire piecewise-linear, continuous phase space trajectory. We show how this is done in the following section.

2 Time-Step Selection Formula

Consider an autonomous Hamiltonian dynamical system with Hamiltonian function $H(\mathbf{z})$ where $\mathbf{z} = (\mathbf{q}, \mathbf{p})^\top \in \Re^{2n}$ and where $\mathbf{q}, \mathbf{p} \in \Re^n$ are the position and momentum coordinates respectively. Let $\mathbf{J}$ be the skew-symmetric matrix

$$\mathbf{J} = \begin{bmatrix} 0 & \mathbf{I}_n \\ -\mathbf{I}_n & 0 \end{bmatrix}$$

where $\mathbf{I}_n$ is the $n \times n$ identity matrix. In symplectic form, Hamilton's equations of motion are given by

$$\frac{d\mathbf{z}}{dt} = \mathbf{J} H_{\mathbf{z}} \tag{1}$$

where $H_{\mathbf{z}}$ is the gradient vector of H [2]. (See [7] for an explanation of symplectic notation in the context of linear Hamiltonian systems.) We will describe a variable step midpoint scheme for discretizing equation (1). First, however, it is convenient to introduce notation for representing piecewise-linear, continuous trajectories.

Assume the points t_k, $k = 0, 1, \cdots N$ partition the interval $[t_0, t_N]$ into N intervals each of length h_k. Assume also that $\hat{\mathbf{z}} : [t_0, t_N] \longrightarrow \Re^{2n}$ is a piecewise-linear, continuous, phase space trajectory as shown in Figure 1. Define $\mathbf{z}^{(k)} = \hat{\mathbf{z}}(t_k)$ to be the vertices of $\hat{\mathbf{z}}(t)$. Clearly, $\hat{\mathbf{z}}(t)$ is completely

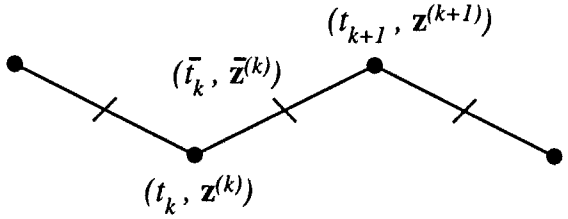


Figure 1: A piecewise-linear, continuous trajectory $\hat{\mathbf{z}}(t)$.

determined by its vertices $\mathbf{z}^{(k)}$.

Define

$$\overline{\mathbf{z}}^{(k)} = \frac{\mathbf{z}^{(k+1)} + \mathbf{z}^{(k)}}{2} \tag{2}$$

$$\overline{\mathbf{z}}'^{(k)} = \frac{\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)}}{h_k} \tag{3}$$

Since the trajectory $\hat{\mathbf{z}}(t)$ is piecewise-linear, it can be expressed in terms of the values of $\overline{\mathbf{z}}^{(k)}$ and $\overline{\mathbf{z}}'^{(k)}$ in the following way.

$$\hat{\mathbf{z}}(t) = \begin{cases} \overline{\mathbf{z}}^{(k)} + \overline{\mathbf{z}}'^{(k)}(t - \bar{t}_k) & t_k \leq t < t_{k+1} \quad k = 0, 1, \cdots N-1 \\ \mathbf{z}^{(N)} & t = t_N \end{cases} \tag{4}$$

where

$$\bar{t}_k = \frac{t_{k+1} + t_k}{2}$$

We now discretize Hamilton's equation using the variable step midpoint scheme

$$\frac{\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)}}{h_k} = \mathbf{J} H_{\mathbf{z}}\left(\frac{\mathbf{z}^{(k+1)} + \mathbf{z}^{(k)}}{2}\right) \tag{5}$$

The midpoint scheme (5) determines a piecewise-linear, continuous phase space trajectory $\hat{\mathbf{z}}(t)$. Using (2) and (3) this midpoint scheme can be expressed more compactly as

$$\overline{\mathbf{z}}'^{(k)} = \mathbf{J} H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)}) \tag{6}$$

For autonomous Hamiltonian systems, the Hamiltonian function $H(\mathbf{z})$ is conserved along the trajectory determined by Hamilton's equations. We use this fact to determine the values of the time-steps h_k by trying to conserve the Hamiltonian function along each linear segment of the piecewise-linear, continuous trajectory $\hat{\mathbf{z}}(t)$ determined by (6). Define

$$\hat{H}(t) = H(\hat{\mathbf{z}}(t)) \tag{7}$$

As a measure of our success in conserving $H(\mathbf{z})$ along the trajectory $\hat{\mathbf{z}}(t)$ we will use the error function

$$e(h_0, h_1, \ldots h_{N-1}) = \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \left(\hat{H}(t) - \hat{H}(\bar{t}_k)\right)^2 dt \tag{8}$$

Our strategy then will be to try to choose values of h_k which minimize $e(h_0, h_1, \ldots h_{N-1})$, but first we obtain an approximation for $e(h_0, h_1, \ldots h_{N-1})$.

For $t_k < t < t_{k+1},\ k = 0, 1, \cdots N-1$ we have the Taylor series expansions

$$\hat{H}(t) = \hat{H}(\bar{t}_k) + \hat{H}'(\bar{t}_k)(t - \bar{t}_k) + \frac{1}{2}\hat{H}''(\bar{t}_k)(t - \bar{t}_k)^2 + \mathcal{O}\left((t - \bar{t}_k)^3\right) \tag{9}$$

Using (7) and the chain rule to expand $\hat{H}'(\bar{t}_k)$ and using equation (6) to substitute for $\overline{\mathbf{z}}'^{(k)}$ we have

$$\begin{aligned} \hat{H}'(\bar{t}_k) &= H_{\mathbf{z}}(\hat{\mathbf{z}}(\bar{t}_k))^{\mathsf{T}} \hat{\mathbf{z}}'(\bar{t}_k) \\ &= H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)})^{\mathsf{T}} \overline{\mathbf{z}}'^{(k)} \\ &= H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)})^{\mathsf{T}} \mathbf{J}\, H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)}) \\ &= 0 \end{aligned} \tag{10}$$

Similarly, expanding $\hat{H}''(\bar{t}_k)$ we have

$$\begin{aligned} \hat{H}''(\bar{t}_k) &= (\hat{\mathbf{z}}'(\bar{t}_k))^{\mathsf{T}} H_{\mathbf{zz}}(\hat{\mathbf{z}}(\bar{t}_k))\ (\hat{\mathbf{z}}'(\bar{t}_k)) + H_{\mathbf{z}}(\hat{\mathbf{z}}(\bar{t}_k))^{\mathsf{T}} \hat{\mathbf{z}}''(\bar{t}_k) \\ &= \left(\overline{\mathbf{z}}'^{(k)}\right)^{\mathsf{T}} H_{\mathbf{zz}}(\overline{\mathbf{z}}^{(k)}) \left(\overline{\mathbf{z}}'^{(k)}\right) \\ &= \left(\mathbf{J} H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)})\right)^{\mathsf{T}} H_{\mathbf{zz}}(\overline{\mathbf{z}}^{(k)}) \left(\mathbf{J} H_{\mathbf{z}}(\overline{\mathbf{z}}^{(k)})\right) \\ &= \psi(\overline{\mathbf{z}}^{(k)}) \end{aligned} \tag{11}$$

where

$$\psi(\mathbf{z}) = (\mathbf{J} H_{\mathbf{z}})^{\mathsf{T}} H_{\mathbf{zz}} (\mathbf{J} H_{\mathbf{z}}) \tag{12}$$

Using (10) and (11) to substitute for $\hat{H}'(\bar{t}_k)$ and $\hat{H}''(\bar{t}_k)$ in (9) we have

$$\hat{H}(t) = \hat{H}(\bar{t}_k) + \frac{1}{2}\psi(\overline{\mathbf{z}}^{(k)})\,(t - \bar{t}_k)^2 + \mathcal{O}\left((t - \bar{t}_k)^3\right), \quad t_k < t < t_{k+1} \tag{13}$$

From (13) we obtain the following third order approximation for $e(h_0, h_1, \ldots h_{N-1})$.

$$\begin{aligned} e(h_0, h_1, \ldots h_{N-1}) &= \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \left(\hat{H}(t) - \hat{H}(\bar{t}_k)\right)^2 dt \\ &\approx \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} \left(\frac{1}{2}\psi(\overline{\mathbf{z}}^{(k)})\,(t - \bar{t}_k)^2\right)^2 dt \\ &= \sum_{k=0}^{N-1} \frac{1}{4}\psi^2(\overline{\mathbf{z}}^{(k)}) \int_{t_k}^{t_{k+1}} (t - \bar{t}_k)^4\, dt \\ &= \frac{1}{320} \sum_{k=0}^{N-1} \psi^2(\overline{\mathbf{z}}^{(k)})\, h_k^5 \end{aligned} \tag{14}$$

We now determine the values of h_k which minimize (14) subject to the constraint

$$\sum_{k=0}^{N-1} h_k = t_N - t_0 \tag{15}$$

(This constraint is necessary to prevent all the values of h_k from being zero.) Using the Lagrange multiplier μ, we define the objective function

$$f(h_0, h_1, \ldots h_{N-1}, \mu) = \frac{1}{320} \sum_{k=0}^{N-1} \psi^2(\overline{\mathbf{z}}^{(k)})\, h_k^5 + \mu \left(t_N - t_0 - \sum_{k=0}^{N-1} h_k \right) \tag{16}$$

Setting the partial derivatives of $f(h_0, h_1, \ldots h_{N-1}, \mu)$ to zero results in the equations

$$\frac{1}{64} \psi^2(\overline{\mathbf{z}}^{(k)}) h_k^4 - \mu = 0 \tag{17}$$

$$t_N - t_0 - \sum_{k=0}^{N-1} h_k = 0 \tag{18}$$

If we assume that the initial time-step h_0 is specified, we can use equation (17) with $k = 0$ to determine the value of μ. This value for μ can then be used in equation (17) for $k > 0$ to obtain the following time-step selection formula

$$h_k = h_0 \sqrt{\frac{\psi(\overline{\mathbf{z}}^{(0)})}{\psi(\overline{\mathbf{z}}^{(k)})}} \tag{19}$$

where $\psi(\mathbf{z})$ is given by (12).

Clearly, the size of the time-steps, h_k, are determined by the initial time-step h_0 and the behavior of $\psi(\mathbf{z})$. For the simple harmonic oscillator with Hamiltonian function $H(\mathbf{z}) = H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2$, we have $\psi(\mathbf{z}) = \psi(q,p) = p^2 + q^2 = 2H(\mathbf{z})$. Since $H(\mathbf{z})$ is constant along the exact trajectory, we should expect that for small initial time-steps, $\psi(\mathbf{z})$ is nearly constant along the approximate trajectory. Thus, for the simple harmonic oscillator, we should expect the time-step formula to yield nearly uniform step sizes. A more detailed analysis of the behavior of $\psi(\mathbf{z})$ is given in [10].

3 Simulation Results

The time-step formula derived in the previous section was implemented in a simple predictor/corrector algorithm and applied to Kepler's problem with

the parameter values given in [1]. The Hamiltonian function is

$$H(\mathbf{z}) = H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

The initial conditions used are

$$q_1 = 1 - e, \quad q_2 = 0, \quad p_1 = 0, \quad p_2 = \sqrt{\frac{1+e}{1-e}}$$

where $e = 0.6$ is the eccentricity of the resulting configuration space orbit. With these parameters, the exact orbit has a period of 2π.

The predictor/corrector scheme used is outline in Figure 2. (Note the use of the abbreviation $H_{\mathbf{z}}^{(k+\frac{1}{2})}$ for $H_{\mathbf{z}}((\mathbf{z}^{(k+1)}+\mathbf{z}^{(k)})/2)$.) Starting with the values of h_k and $\mathbf{z}^{(k)}$, a second order Runge-Kutta scheme is used to "predict" the value of $\mathbf{z}^{(k+1)}$. The Hessian matrix $H_{\mathbf{zz}}$ is computed and used to evaluate $\psi_{k+\frac{1}{2}} = \psi((\mathbf{z}^{(k+1)}+\mathbf{z}^{(k)})/2)$ (This Hessian matrix is also used by the midpoint corrector.) The value of $\psi_{k+\frac{1}{2}}$ is used to compute the new step size h_{k+1} which is then used to "correct" the predicted value for $\mathbf{z}^{(k+1)}$. The correction step is accomplished by applying one iteration of Newton's method to the implicit equations of the midpoint scheme with the predicted value of $\mathbf{z}^{(k+1)}$ used as an initial guess.

$$\begin{aligned} \mathbf{z}^{(k+\frac{1}{2})} &= \mathbf{z}^{(k)} + \frac{1}{2}h_k \mathbf{J} H_{\mathbf{z}}^{(k)} \\ \mathbf{z}^{(k+1)} &= \mathbf{z}^{(k)} + h_k \mathbf{J} H_{\mathbf{z}}^{(k+\frac{1}{2})} \end{aligned} \qquad \text{Second order Runge-Kutta predictor.}$$

$$h_{k+1} = h_0 \sqrt{\frac{\psi_0}{\psi_{k+\frac{1}{2}}}} \qquad \text{Step size adjustment.}$$

$$\mathbf{z}^{(k+1)} - \mathbf{z}^{(k)} - h_{k+1} \mathbf{J} H_{\mathbf{z}}^{(k+\frac{1}{2})} = 0 \qquad \text{Midpoint corrector (one iteration).}$$

Figure 2: Predictor/Corrector Algorithm

For comparison, a fixed step version of the predictor/corrector algorithm was implemented by removing the time-step adjustment portion of the algorithm shown in Figure 2. For each scheme, initial time-steps were chosen

so that the total number of function evaluations were the same, about 50 time-steps per orbit for a total of 1,000 steps for both fixed and variable step implementations.

Figure 3 shows that the variable-step scheme significantly reduces errors in the Hamiltonian function. Not only is the error in the Hamiltonian along each orbit much less, but there also appears to be less drift in the Hamiltonian over time. A question that might be asked at this point is what effect does reducing the error in the Hamiltonian have on the discretization errors in the position and momentum coordinates. Figure 4 and Figure 5 seem to indicated that the peak errors in the position and momentum coordinates are not significantly reduced by the variable-step scheme. However, the figures show that the errors for the variable step scheme are more regular than those of the fixed step scheme.

Figure 6 shows that the configuration space orbits of the variable step scheme are significantly more accurate than those of the fixed step scheme. The orbits of the variable step scheme have a much lower precession rate.

For even moderate eccentricities, the time-step ratios h_k/h_0 can change by more than an order of magnitude. For orbits with eccentricity $e = 0.6$, Figure 7 shows that the largest time-step is more than 20 times as large as the smallest time-step. For larger eccentricities, the time-step ratios h_k/h_0 can change by several orders of magnitude. The time-step formula given by equation (19) fails in situations where $\psi(\mathbf{z}) = 0$. Examples of such situations are given in [12]. Strategies need to be developed for limiting the size of time-steps when the value of $\psi(\mathbf{z})$ is near zero.

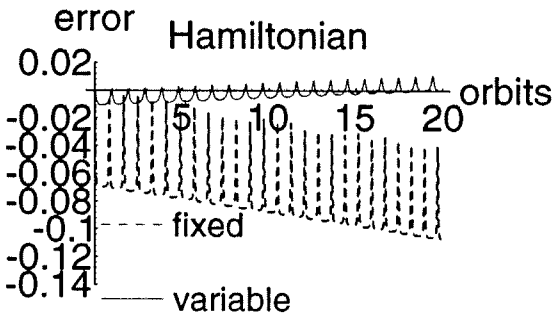
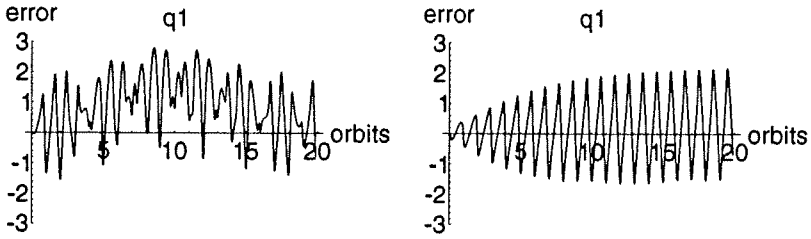
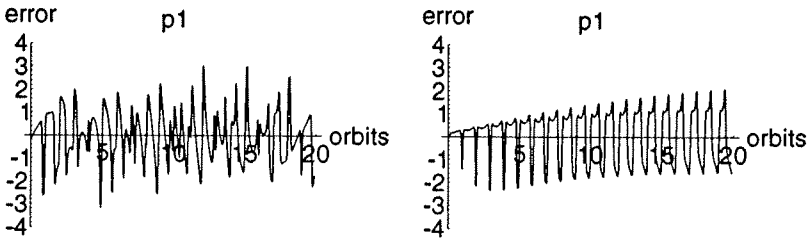


Figure 3: A comparison of errors in the Hamiltonian function.



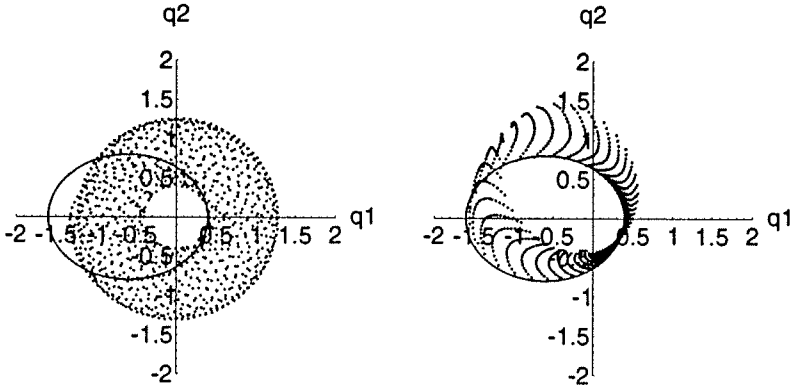
(a) fixed time-step (b) variable time-step

Figure 4: A comparison of the errors in q_1.



(a) fixed time-step (b) variable time-step

Figure 5: A comparison of the errors in p_1.



(a) fixed time-step (b) variable time-step

Figure 6: A 20 orbit comparison with the exact orbit. Only the vertices of the trajectories of each scheme are shown.

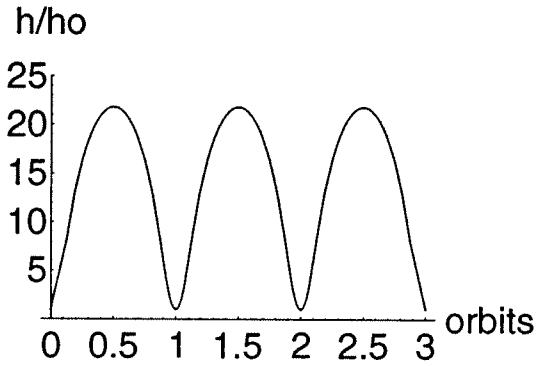


Figure 7: Time-step ratios evaluated along the exact trajectory.

4 Conclusions

While we have not shown rigorously that the values of h_k determined by the time-step selection formula (19) actually minimize the error in the Hamiltonian along piecewise-linear trajectories, computer experiments for the Kepler problem show that this formula works well in practise. The observed improvement in the regularity of the resulting position and momentum coordinates may be desirable in applications of statistical mechanics where accurate time dependent trajectories are not of primary importance.

By using an extended phase space formulation, it should be possible to apply the variable-step midpoint scheme described in this paper to nonautonomous Hamiltonian systems. For nonautonomous systems, however, the energy is no longer conserved, but the extended phase Hamiltonian continues to be conserved.

Other methods exist for Newtonian potential systems which exploit conservation of energy. Velocities can be scaled to conserve energy [8]. Likewise, it is possible to scale forces to conserve energy [9]. Further work needs to be done comparing the merits of the variable-step method described here to such methods. Further work is also need to determine how the method affects other properties of Hamiltonian systems such as symplecticity [6, 13] and time-symmetry [3].

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