Variable time step integration with symplectic methods

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Abstract

Symplectic methods for Hamiltonian systems are known to have favourable properties concerning long-time integrations (no secular terms in the error of the energy integral, linear error growth in the angle variables instead of quadratic growth, correct qualitative behaviour) if they are applied with constant step sizes, while all of these properties are lost in a standard variable step size implementation. In this article we present a "meta-algorithm" which allows us to combine the use of variable steps with symplectic integrators, without destroying the above mentioned favourable properties. We theoretically justify the algorithm by a backward error analysis, and illustrate its performance by numerical experiments.

Keywords: Hamiltonian systems, symplectic integration, variable step sizes, backward error analysis, Kepler's problem, Verlet scheme

1 Introduction

Hamiltonian systems of ordinary differential equations arise in many applications (e.g., mechanics, astrophysics, molecular dynamics) and are of the form

$$p' = -H_q(p,q), \qquad q' = H_p(p,q), \tag{1}$$

where $H(p_1,\ldots,p_d,q_1,\ldots,q_d)$ denotes the Hamiltonian function and H_p, H_q are vectors of partial derivatives. Such systems have the properties that (a) the Hamiltonian function is a first integral of the system and (b) its flow is a symplectic transformation, i.e., it preserves the differential 2-form $dp \wedge dq$.

In this article we consider the numerical integration of Hamiltonian systems by symplectic one-step methods, i.e., methods for which the numerical flow

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$(p_1, q_1) = \Phi_h(p_0, q_0)$ is for all sufficiently small $h > 0$ a symplectic transformation. For such methods, the numerical solution can be formally interpreted as the exact solution of a perturbed Hamiltonian system (backward error analysis), and thus preserves the qualitative features of the original system.

It has been observed numerically by Gladman, Duncan & Candy [2] and by Calvo & Sanz-Serna [1] that symplectic integrators, when used with variable step sizes, lose their favourable properties for long-time integrations and are no longer superior to standard non-symplectic methods. It appeared that symplectic methods could not solve efficiently problems where variable steps are indispensable (e.g., Kepler's problem with high eccentricity), and McLachlan & Scovel [10] presented as an open problem to "develop variable time step symplectic integrators so that they are competitive ... with standard methods ... while retaining the good long-time behaviour of constant time-step symplectic methods".

There are several attempts to overcome the difficulties mentioned above. Skeel & Biesiadecki [14] decompose the vector field and integrate over a basic time step h different parts with different step sizes (multiple-time-step method), so that the overall method defines a symplectic transformation. Since the basic step size is not altered, its long-time behaviour is like that of a constant step size method (similar as if we apply a symplectic method with steps of alternating size h and $2h$). In the case where the system is reversible and the method symmetric, several step size strategies have been found that retain the good long-time behaviour. Such so-called reversible step size strategies have been proposed and studied by Hut, Makino & McMillan [7], Stoffer [18], Hairer & Stoffer [5], and Huang & Leimkuhler [6].

Our approach of this article is conceptually completely different. We do not make any reversibility assumptions on the system, and the approach works for all (not necessarily symmetric) one-step methods. The idea is to add small perturbations to the discretization, such that the qualitative behaviour for long-time integrations is re-established, without affecting the order of convergence (Sect. 2). The algorithm is theoretically justified in Sect. 3, and practical considerations for an implementation together with numerical experiments are discussed in the final sections.

2 Symplectic Meta-Algorithm for Variable Step Sizes

We attack the problem by considering a time transformation $t \leftrightarrow \tau$ satisfying $dt/d\tau = s(p(\tau), q(\tau))$ such that the system (1) becomes

$$\begin{pmatrix} p \\ q \end{pmatrix}' = s(p,q) \begin{pmatrix} -H_q(p,q) \\ H_p(p,q) \end{pmatrix} . \tag{2}$$

Applying a numerical method with constant step size ε to (2) yields approximations (p_n, q_n) to $(p(t_n), q(t_n))$, where $t_{n+1} - t_n \approx \varepsilon\, s(p_n, q_n)$. It has been pointed out by Stoffer [17], [18] and Skeel & Gear [15] that the system (2) can be Hamiltonian only if $s(p, q)$ is constant along solutions of (1), what makes this approach unattractive.

The new idea, proposed here, is the following: suppose that we want to integrate the system (1) with steps of size

$$h = \varepsilon\, s(p, q, \varepsilon), \tag{3}$$

where $s(p, q, \varepsilon) > 0$ is a state-dependent given function and $\varepsilon > 0$ is a small parameter. Then we consider, for a fixed initial value (p_0, q_0) with $H_0 = H(p_0, q_0)$, the *new Hamiltonian*

$$K(p, q, \varepsilon) = s(p, q, \varepsilon)\Big(H(p, q) - H_0\Big), \tag{4}$$

and the corresponding Hamiltonian system

$$\begin{aligned} p' &= -s(p, q, \varepsilon) H_q(p, q) - s_q(p, q, \varepsilon)(H(p, q) - H_0) \\ q' &= s(p, q, \varepsilon) H_p(p, q) + s_p(p, q, \varepsilon)(H(p, q) - H_0). \end{aligned} \tag{5}$$

Compared to (2) we have introduced a perturbation, which vanishes on the solution of (1) passing through (p_0, q_0), but which makes the system Hamiltonian.

Lemma 1 *Let $(p(t), q(t))$ and $(P(t), Q(t))$ be the solutions of (1) and (5), respectively, both with initial values (p_0, q_0). Then, it holds*

$$P(t) = p(\alpha(t, \varepsilon)), \qquad Q(t) = q(\alpha(t, \varepsilon))$$

where $\alpha(t, \varepsilon) = \int_0^t s(P(\tau), Q(\tau), \varepsilon)\, d\tau.$

Proof. This follows from the fact that along the considered solution of (5) we have $K(P(t), Q(t)) = K(p_0, q_0) = 0$, so that $H(P(t), Q(t)) = H_0$. Therefore, $(P(t), Q(t))$ and $(p(\alpha(t, \varepsilon)), q(\alpha(t, \varepsilon)))$ satisfy the same differential equation (2) with the same initial values. $\square$

We are now ready to present the principle of our algorithm.

Algorithm 1 *Apply a symplectic one-step method with constant step size ε to the Hamiltonian system (5), augmented by $t' = s(p, q, \varepsilon)$. This yields numerical approximations (p_n, q_n) to $(P(n\varepsilon), Q(n\varepsilon))$, and t_n to $\alpha(n\varepsilon, \varepsilon)$. Hence we have*

$$p_n \approx p(\alpha(n\varepsilon, \varepsilon)), \qquad q_n \approx q(\alpha(n\varepsilon, \varepsilon)),$$

where $(p(t), q(t))$ is the solution of the original system (1).

Remark 2 [2] *Time transformations such as in Eq. (4) are already used in classical mechanics for an analytic treatment of Hamiltonian systems. They date back to the work of Levi-Civita ([8], page 313, and [9], pages 120 and 134), where the three body problem is considered with the special time transformation $dt/d\tau = r = \|q\|$. Levi-Civita calls this the "Darboux-Sundman transformation" (see Sundman [16]).*

Zare & Szebehely [20] consider such time transformations for numerical purposes. These authors are not interested in symplectic methods, but they consider the additional term in Eq. (5) as control term stabilizing the numerical integration. Their favourite choice of $s(p, q, \varepsilon)$ is the inverse of the Lagrange function, for which the partial derivatives s_p and s_q are already known. Waldvogel & Spirig [19] apply the transformations proposed by Levi-Civita to Hill's lunar problem and solve the transformed equations by composition methods in order to preserve the symplectic structure.

Remark 3 *The idea of considering the Hamiltonian (4) for a symplectic variable step size integration has been found independently by S. Reich [12].*

3 Backward Error Analysis

The favourable long-time behaviour of symplectic methods for Hamiltonian systems, in the case of constant step sizes, can be understood by a backward error analysis (see e.g., Sanz-Serna & Calvo [13] or Hairer & Lubich [4]). Although our algorithm yields numerical approximations on a non-equidistant grid, it can be considered as a fixed step size, symplectic method applied to a different Hamiltonian system. This interpretation allows us to apply the standard results on backward error analysis. In particular, we have the following result.

Theorem 4 *Consider the Hamiltonian system (1) and let (p_n, q_n) be the numerical solution obtained by Algorithm 1 with a symplectic one-step method. Then, there exist a perturbed Hamiltonian*

$$\widetilde{H}(p, q, \varepsilon) = H(p, q) + \varepsilon H_1(p, q) + \varepsilon^2 H_2(p, q) + \ldots, \tag{6}$$

and a perturbed time transformation

$$\widetilde{\alpha}(t, \varepsilon) = \alpha(t, \varepsilon) + \varepsilon\alpha_1(t) + \varepsilon^2\alpha_2(t) + \ldots \tag{7}$$

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[2] We are grateful to W.M. Seiler (University Karlsruhe) and B. Leimkuhler (University of Kansas) for drawing our attention to these references.

with $\alpha(t,\varepsilon)$ *from Lemma 1, such that (formally)*

$$p_n = \tilde{p}(\tilde{\alpha}(n\varepsilon,\varepsilon)), \qquad q_n = \tilde{q}(\tilde{\alpha}(n\varepsilon,\varepsilon)),$$

where $\tilde{p}(t), \tilde{q}(t)$ *is the exact solution of*

$$\tilde{p}' = -\widetilde{H}_q(\tilde{p},\tilde{q}), \qquad \tilde{q}' = \widetilde{H}_p(\tilde{p},\tilde{q}).$$

If the underlying one-step method is of order r*, the perturbations in (6) and (7) start with the* ε^r*-terms.*

Proof. For the symplectic method applied with constant step size ε to the Hamiltonian system (5), standard backward error analysis yields the existence of a perturbed Hamiltonian

$$\widetilde{K}(p,q,\varepsilon) = K(p,q,\varepsilon) + \varepsilon K_1(p,q) + \varepsilon^2 K_2(p,q) + \ldots$$

(without loss of generality we may assume that $K_j(p_0,q_0) = 0$ for all j), such that formally

$$p_n = \widetilde{P}(n\varepsilon), \qquad q_n = \widetilde{Q}(n\varepsilon),$$

where $\widetilde{P}(t), \widetilde{Q}(t)$ is the exact solution of the Hamiltonian system corresponding to $\widetilde{K}(p,q,\varepsilon)$ with initial values (p_0,q_0). We now define

$$\widetilde{H}(p,q,\varepsilon) := \widetilde{K}(p,q,\varepsilon)/s(p,q,\varepsilon) + H_0.$$

The solution $\tilde{p}(t), \tilde{q}(t)$ of the corresponding Hamiltonian system satisfies by Lemma 1

$$\widetilde{P}(t) = \tilde{p}(\tilde{\alpha}(t,\varepsilon)), \qquad \widetilde{Q}(t) = \tilde{q}(\tilde{\alpha}(t,\varepsilon)),$$

where $\tilde{\alpha}(t,\varepsilon) := \int_0^t s(\widetilde{P}(\tau),\widetilde{Q}(\tau),\varepsilon)\,d\tau = \alpha(t,\varepsilon) + \varepsilon\alpha_1(t) + \ldots\ .$ $\Box$

4 Practical Considerations for Separable Hamiltonians

In the case of separable Hamiltonians $H(p,q) = T(p) + V(q)$, it is known that there exist *explicit* symplectic integrators. However, the transformed Hamiltonian (4) is no longer separable. We shall see in this section that the advantage of explicit symplectic integrators can nevertheless be preserved. We illustrate this for the important case of Hamiltonian functions

$$H(p,q) = \frac{1}{2}p^T M^{-1} p + V(q), \tag{8}$$

where M is a constant symmetric matrix.

4.1 Symplectic Euler Method with q-Dependent Step Size Function

The most simple symplectic integration scheme is the combination of the implicit Euler method (for the p-variables) and the explicit Euler method (for the q-variables). If we consider step size functions of the form $h = \varepsilon s(q, \varepsilon)$, where s is independent of p, this method, when applied to the system (5) with Hamiltonian (8), reads

$$
\begin{aligned}
p_1 &= p_0 - \varepsilon s(q_0, \varepsilon) V_q(q_0) - \varepsilon s_q(q_0, \varepsilon)\left(\tfrac{1}{2} p_1^T M^{-1} p_1 + V(q_0) - H_0 \right) \\
q_1 &= q_0 + \varepsilon s(q_0, \varepsilon) M^{-1} p_1
\end{aligned} \tag{9}
$$

and yields an approximation at $t_1 = t_0 + \varepsilon s(q_0, \varepsilon)$. We get a quadratic equation in p_1, which can be solved as follows: we consider the norm $\|p\|_M^2 := p^T M^{-1} p$ and compute the scalar quantity $\beta := p_1^T M^{-1} p_1 = \|p_1\|_M^2$ from the relation

$$
\beta = \|p_0 - \varepsilon s(q_0, \varepsilon) V_q(q_0) - \varepsilon s_q(q_0, \varepsilon)(\beta/2 + V(q_0) - H_0)\|_M^2 .
$$

This scalar quadratic equation can easily be solved for β. Then, the numerical solution p_1, q_1 is obtained in an explicit manner from (9).

4.2 Symplectic Euler Method with Arc-Length Parametrization

For general step size functions $h = \varepsilon s(p, q, \varepsilon)$ the symplectic Euler method, applied to (5), reads

$$
\begin{aligned}
p_1 &= p_0 - \varepsilon s(p_1, q_0, \varepsilon) V_q(q_0) - \varepsilon s_q(p_1, q_0, \varepsilon)\left(\tfrac{1}{2} p_1^T M^{-1} p_1 + V(q_0) - H_0\right) \\
q_1 &= q_0 + \varepsilon s(p_1, q_0, \varepsilon) M^{-1} p_1 + \varepsilon s_p(p_1, q_0, \varepsilon)\left(\tfrac{1}{2} p_1^T M^{-1} p_1 + V(q_0) - H_0\right)
\end{aligned} \tag{10}
$$

Here, the first equation is implicit in p_1. However, if the function $s(p, q, \varepsilon)$ only depends on q and on $p^T M^{-1} p$, we again can first solve a scalar equation for $\beta := p_1^T M^{-1} p_1$ and the remaining computations are explicit. Such step size functions include the arc-length parametrization of the solution (see e.g., McLeod & Sanz-Serna [11] and Huang & Leimkuhler [6]), where

$$
s(p, q, \varepsilon) = \left(p^T M^{-1} p + V_q(q)^T M^{-1} V_q(q) \right)^{-1/2}. \tag{11}
$$

We have chosen the norm $\| \cdot \|_M$ instead of the Euclidean norm, because it leaves the expression (11) invariant with respect to linear coordinate changes.

Since the Hamiltonian (8) is constant along solutions of the system, the step size function of Eq. (11) can be replaced by the p-independent function

$$s(q,\varepsilon) = \Big(2(H_0 - V(q)) + V_q(q)^T M^{-1} V_q(q)\Big)^{-1/2}. \tag{12}$$

Numerical experiments revealed that the use of (11) and (12) give nearly identical results.

4.3 Verlet Scheme with q-Dependent Step Size Function

One of the most important symplectic integration schemes is the Störmer or Verlet method, which is equivalent to the 2-stage Lobatto IIIA-IIIB pair. In contrast to the method of Eq. (10), it is also symmetric. This property is important for the integration of time reversible problems. Applied to the system (5) with $H(p,q)$ given by (8) and with p-independent function s, it is of the form

$$\begin{aligned}
p_{n+1/2} &= p_n - \frac{\varepsilon}{2} s(q_n,\varepsilon) V_q(q_n) - \frac{\varepsilon}{2} s_q(q_n,\varepsilon)(H(p_{n+1/2},q_n) - H_0)\\
q_{n+1} &= q_n + \frac{\varepsilon}{2}(s(q_n,\varepsilon) + s(q_{n+1},\varepsilon)) M^{-1} p_{n+1/2}\\
p_{n+1} &= p_{n+1/2} - \frac{\varepsilon}{2} s(q_{n+1},\varepsilon) V_q(q_{n+1}) - \frac{\varepsilon}{2} s_q(q_{n+1},\varepsilon)(H(p_{n+1/2},q_{n+1}) - H_0).
\end{aligned} \tag{13}$$

The first equation is equivalent to that of (9), and can be solved for $p_{n+1/2}$ as explained in Sect. 4.1. The second equation of (13) is implicit in q_{n+1}. However, it is sufficient to solve the scalar equation

$$\gamma = s\Big(q_n + \frac{\varepsilon}{2}(s(q_n,\varepsilon) + \gamma) M^{-1} p_{n+1/2}, \varepsilon\Big)$$

for $\gamma := s(q_{n+1},\varepsilon)$. This can be done efficiently by Newton iterations, because the derivative $s_q(p,q,\varepsilon)$ is available. The last equation in (13) is explicit. The scheme (13) gives approximations at t_n, where $t_{n+1} = t_n + \varepsilon(s(q_n,\varepsilon) + s(q_{n+1},\varepsilon))/2$.

Composition methods (see e.g., [13]) are an interesting tool for the derivation of higher order integration methods. Since they are based on the second order Verlet scheme, there is no obstacle in applying them with variable step sizes in the form of Eq. (13).

5 Numerical Experiments

Here we study different choices of step size functions $s(p,q,\varepsilon)$, and we compare the algorithm (13) to the so-called adaptive Verlet method of Huang & Leimkuhler [6].

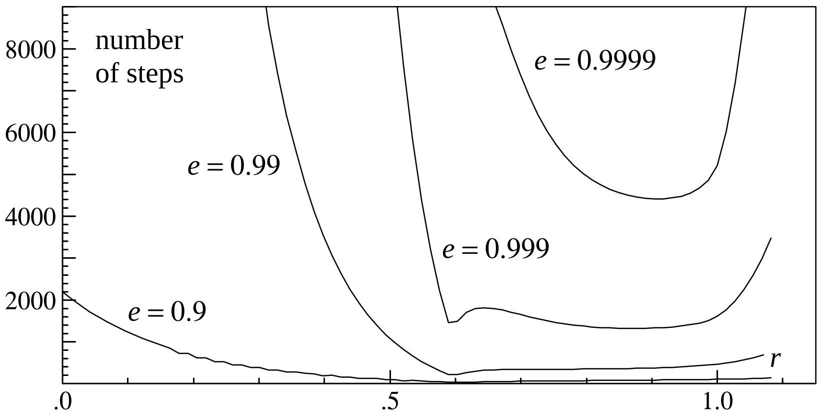

Fig. 1. Minimum number of steps as function of r

5.1 Kepler's Problem

We consider Kepler's problem, for which the Hamiltonian is

$$H(p,q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \tag{14}$$

and we take initial values

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{15}$$

such that in the (q_1, q_2)-plane the solution is an ellipse with eccentricity e. The movement is fast when the point (q_1, q_2) is close to the origin. Hence, it is natural to take small time steps when $q_1^2 + q_2^2$ is small, and large time steps when $q_1^2 + q_2^2$ is large. We thus consider

$$s(q, \varepsilon) = (q_1^2 + q_2^2)^r \tag{16}$$

as step size function. For many different values of r between 0 and 1.1 we have integrated Kepler's problem on the interval $[0, 2\pi]$ with the symplectic variable step size Verlet scheme (13). We have adapted the value of ε in such a way that the maximal error in the Hamiltonian is approximately equal to 0.01. Fig. 1 shows the necessary work (i.e., number of steps to achieve this goal) as function of r. We see that the constant step size implementation, which corresponds to $r = 0$, does not give satisfactory results at all. The optimal value of r lies somewhere between 0.5 and 1, and is closer to 1 for larger eccentricities.

In Table 1 these numbers are explicitly given for some particular values of r. We have also included the results of the arclength parametrization (12). They are similar to those obtained with $r = 1$, because the function of Eq. (12) behaves like $\|q\|^2$ for small $\|q\|$. The results of a similar experiment, where

Table 1
Minimum number of steps, such that the error in the Hamiltonian is ≤ 0.01

	eccentricity	$e = 0.9$	$e = 0.99$	$e = 0.999$	$e = 0.9999$
	minimum	34	215	1323	4412
Method	$r = 0$	2192	229479	—	—
(13)	$r = 1$	110	469	1608	5210
	arclength	116	439	1761	6673
Method	$r = 1$	249	1440	6037	22825
(17)	arclength	211	1264	5484	21205

Table 2
Minimum number of steps, such that the error in the solution is ≤ 0.1

	eccentricity	$e = 0.684$	$e = 0.900$	$e = 0.968$	$e = 0.990$
	$r = 0$	875	29483	920751	—
Method	$r = 1$	123	688	3785	21620
(13)	arclength	172	1140	6449	36418
Method	$r = 1$	135	2244	18024	129698
(17)	arclength	138	1964	15938	116441

we consider the error in the solution instead of the error in the Hamiltonian, are shown in Table 2. We give the minimum number of steps, such that the Euclidean norm of the error in the position and momentum variables is not larger than 0.1 (on the whole integration interval). The reference solution is obtained by an eighth order explicit Runge-Kutta method with $Tol = 10^{-14}$. In Tables 1 and 2 we have also included the results of the adaptive Verlet scheme (see (17) below).

Fig. 2 illustrates how the different step size functions influence the position of the output points. We have chosen $e = 0.6$. The picture to the left uses the function of Eq. (12), in the middle we use $s(q, \varepsilon) = 1/\sqrt{H_0 - V(q)}$ (arclength parametrization in the q-variables only), and the picture to the right corresponds to $s(q, \varepsilon) = 1$ (constant step size). In each case we have adjusted the parameter ε in such a way that the maximal error in the Hamiltonian is close to 0.023.

5.2 The Adaptive Verlet Method of Huang & Leimkuhler

A variable step size method, closely related to (13), has recently been proposed by Huang & Leimkuhler [6]. It also generalizes the Verlet scheme, and is for separable Hamiltonians (8) and for q-dependent step size functions $s(q, \varepsilon)$ given by

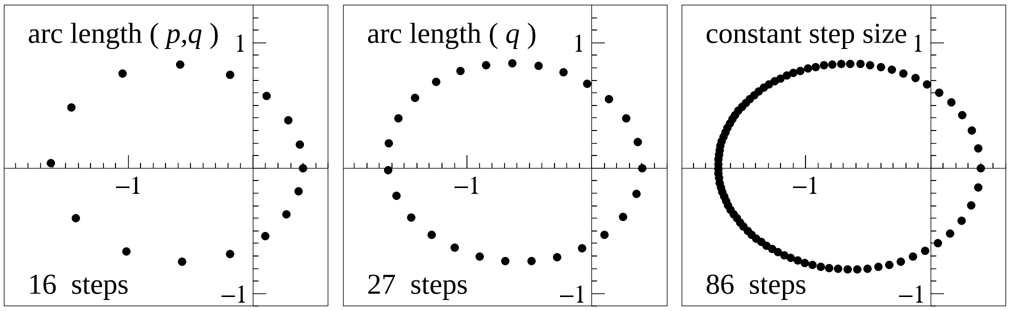

Fig. 2. Various step size strategies for Kepler's problem

$$\begin{aligned}
p_{n+1/2} &= p_n - \frac{\varepsilon}{2}\sigma_{n+1/2} V_q(q_n) \\
q_{n+1} &= q_n + \varepsilon \sigma_{n+1/2} M^{-1} p_{n+1/2} \\
p_{n+1} &= p_{n+1/2} - \frac{\varepsilon}{2}\sigma_{n+1/2} V_q(q_{n+1}),
\end{aligned} \tag{17}$$

where $\sigma_{n+1/2}$ is defined by the recursion

$$\sigma_{1/2} = s(q_0, \varepsilon), \qquad \frac{1}{\sigma_{n+1/2}} + \frac{1}{\sigma_{n-1/2}} = \frac{2}{s(q_n, \varepsilon)}. \tag{18}$$

Both methods, (13) and (17), are symmetric and they preserve the angular momentum (for (13) one has to restrict the step size function such that the system (5) preserves also the angular momentum). Method (17) has the advantage of being explicit. Method (13), on the other hand, is implicit (limited tests revealed that one step of (13) is about three times as expensive as one step of (17) with the same ε), but it retains the symplecticness of the fixed step size Verlet scheme.

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