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The rate of error growth in Hamiltonian-conserving integrators

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1. Introduction

We consider Hamiltonian systems in $\mathbb{R}^{2N}$ of the form

$$\begin{aligned} z_t &= J\nabla H(z), \\ z(0) &= z_0, \end{aligned} \tag{1.1}$$

where J is a skew-symmetric matrix. We assume that there is a set $\Omega \subseteq \mathbb{R}^{2N}$ such that the solutions of (1.1) for $z_0 \in \Omega$ exist and remain in Ω for all $t \in \mathbb{R}^+$. We let $S(\bullet)\bullet\colon \mathbb{R}^+ \times \mathbb{R}^{2N} \mapsto \mathbb{R}^{2N}$ denote the evolution semigroup defined so that $z(t) = S(t)z_0$ and let $dS(z_0, t)$ denote the Jacobian matrix of $S(t)z_0$ with respect to z_0. Note that $S(t)$ is defined for all $t \geq 0$ on Ω. Fundamental to the evolution of (1.1) are the facts that the Hamiltonian is preserved:

(i) $H(S(t)z_0) = H(z_0) = J$, for all $z_0 \in \Omega$, $t \in \mathbb{R}^+$;

and there is a symplectic structure that is preserved:

(ii) $dS(z_0, t)^T J\, dS(z_0, t) = J$, for all $z_0 \in \Omega$, $t \in \mathbb{R}^+$.

We consider approximations of (1.1) computed on a uniform partition of $\mathbb{R}^+$: $t_0 = 0 < t_1 < t_2 < \cdots$ with timestep Δt. Ideally, we would preserve both (i) and (ii) when considering schemes for the numerical solution of (1.1). Unfortunately, except for integrable systems, it is not possible to construct numerical algorithms that enforce (discrete analogs of) (i) and (ii) simultaneously ([18]). Thus, a choice has to be made between algorithms that conserve the *Hamiltonian* and satisfy a discrete analog of (i) (which we call Hamiltonian-conserving algorithms) or algorithms that conserve the

symplectic structure and satisfy a discrete analog of (ii) (known as symplectic algorithms).

In recent years, there has been a proliferation of work on symplectic integrators (see [9], [11], and [17] for a review of the literature) while Hamiltonian-conserving algorithms have received considerably less attention. Essentially, the literature contains three basic arguments put forward in favor of symplectic integrators:

(a) In the neighborhood of an equilibrium point of center type, a symplectic algorithm has stability properties similar to those of (1.1) itself; see [10].
(b) For problems that have a periodic solution with the period determined uniquely by $H(z_0)$, such as Kepler's problem, the first term in a power series expansion of the error in terms of the time step Δt depends linearly on time. In contrast, for generic algorithms for (1.1), the error grows superlinearly with time; see [12], [8], and [17].
(c) The method of the modified equation shows that, for every integer q, there is a Hamiltonian system with Hamiltonian $H^{(q)}(z)$ such that the numerical solution of a symplectic algorithm is an $\mathcal{O}(\Delta t^q)$ approximation of the solution of a system with Hamiltonian $H^{(q)}(z)$. In some sense, this shows that symplectic algorithms "almost" satisfy a property related to (i) above. However, $H^{(q)}$ does not converge to a limit functional as $q \to \infty$; see [11] and the references therein.

Point (a) is certainly of interest. However, Hamiltonian-conserving algorithms have the same property in the plane. Furthermore, there are problems in which Hamiltonian-conserving algorithms have better stability properties than symplectic algorithms ([13], [14], and [5]) because the stability properties of the true solution in the neighborhood of complicated invariant sets, such as relative equilibria, are not necessarily inherited by symplectic algorithms, and symplectic algorithms can blow-up in such situations. Hamiltonian-conserving algorithms appear considerably more robust for such problems [5].

Point (c) is also of interest with possible consequences for the interpretation of data from numerical simulations over long time intervals ([9], [11]). But the asymptotic nature of the result, in terms of powers of Δt, makes it difficult to draw rigorous and definite conclusions.

In this note, we show that (b) is also satisfied by Hamiltonian-conserving methods. Indeed, the result for Hamiltonian-conserving methods is much stronger than for symplectic methods, since the *total* error grows linearly in time, not just the first term in a series expansion of the error in powers of Δt. This result is proved in section 2 and a numerical example is given in section 3. In the same context, we mention an analysis of the rate of propagation of error in energy-conserving schemes for the Korteweg-de-Vries equation ([3]).

Finally, we mention the work of Kirchgraber [7] on the Stiefel-Baumgarte stabilization procedure [15], [2]; this method replaces (1.1) by another ordinary differential equation for which the level sets of the conserved quantities are attractive. In the case where (1.1) is integrable it is then possible to show that application of *any* consistent method to the stabilized system yields an error which grows linearly in time and has the optimal order of convergence in powers of Δt [7]. A similar result holds for some special non-integrable systems, but a power of Δt is lost in the error bound [7]. Note that, in contrast, our analysis applies only to certain conserving methods but does not require transformation of (1.1) into a different problem, which may be hard to implement in practice. Further ramifications of the work of [7] are discussed in Important Remark (iii) following the proof of the Theorem in section 2.

In conclusion, this note is an addition to the growing body of literature which indicates that the relative merits of symplectic and Hamiltonian-conserving algorithms needs further investigation.

2. The result

Our result is motivated by the study of planar Hamiltonian systems near a center and by study of bounded solutions of the two-body Kepler problem. For such systems it is natural to assume that there is a set on which H is smooth with the following property: solutions starting in this set are periodic with period determined solely by the initial value of the Hamiltonian. More precisely:

Assumption 1. *There is an open set* $\Omega \subseteq \mathbb{R}^{2N}$ *such that* $H \in C^\infty(\Omega, \mathbb{R})$. *For any* $z_0 \in \Omega$ *there exists a* $T = T(H(z_0))$ *such that* $S(T)z_0 = z_0$ *and there exists a closed, bounded set* $B_1 \subset \Omega$ *such that* $S(t)z_0 \in B_1$ *for all* $t \geq 0$.

Functional relationships between the period and the Hamiltonian are natural in Hamiltonian systems (see [6]) so that Assumption 1 is not as restrictive as it might first appear.

We recall that the continuity of the semigroup means that if $z_1, z_2 \in \tilde{\Omega}$, a bounded subset of Ω, $\|z_1 - z_2\| \leq \delta$, and $\tau > 0$, then there exists a $C_2 = C_2(\tilde{\Omega}, \tau)$ such that

$$\|S(t)z_1 - S(t)z_2\| \leq C_2\delta, \qquad \forall t \in [0, \tau]. \tag{2.1}$$

Next, we assume that $\mathbb{R}^+$ is partitioned uniformly with time step Δt and let Z_n denote the approximation to $z(n\Delta t)$ for $n \geq 0$, with $Z_0 = z_0$. We introduce the semigroup $S^1_{\Delta t}: \mathbb{R}^{2N} \mapsto \mathbb{R}^{2N}$ that produces the approximation,

$$Z_{n+1} = S^1_{\Delta t} Z_n, \tag{2.2}$$

and we let $S^n_{\Delta t} = S^1_{\Delta t} \bullet \cdots \bullet S^1_{\Delta t}$, n times. We recall that $S^n_{\Delta t} S^m_{\Delta t} = S^{n+m}_{\Delta t}$. We now assume that the numerical method converges with order r on finite time intervals, remains bounded for all time for data taken in a certain set, and conserves the Hamiltonian. More precisely:

Assumption 2. *For any $z_0 \in \tilde{\Omega}$, a closed, bounded subset of Ω, and $\tau \in \mathbb{R}^+$ there exists an integer $r > 0$ and constants $C_1 = C_1(\tilde{\Omega}, \tau)$ and $\Delta t_c = \Delta t_c(\tilde{\Omega}, \tau)$ such that*

$$\left\| S^n_{\Delta t} z_0 - S(n\Delta t) z_0 \right\| \leq C_1 \Delta t^r$$

for all n and Δt with $0 \leq n\Delta t \leq t$ and $0 \leq \Delta t \leq \Delta t_c$. Furthermore, for any $z_0 \in \Omega$ and $\Delta t \in \mathbb{R}^+$ the approximation satisfies $H(S^n_{\Delta t} z_0) = H(z_0)$ for all integers n, and there exists a closed, bounded set $B_2 \subset \Omega$, such that $S^n_{\Delta t} z_0 \in B_2$ for all integers n.

Note that both the true solutions and the numerical approximations are assumed to remain bounded away from the boundary of Ω, where H may fail to be defined, uniformly in time. Our main result is:

Theorem. *Assume that Assumptions 1 and 2 hold. For any $z_0 \in \Omega$, let $T = T(H(z_0))$ be given by Assumption 1 and assume that $\Delta t = T/N$ for some integer N. Then, there exists a closed, bounded set $B \subset \Omega$ such that $S(t)z_0$, $S^n_{\Delta t} z_0 \in B$ for all $t, n \geq 0$. Furthermore, there are constants $C_3 = C_3(B, T)$ and $\Delta t_c = \Delta t_c(B, T)$ such that for any integer $m \geq 0$,*

$$\left\| S^n_{\Delta t} z_0 - S(n\Delta t) z_0 \right\| \leq (1 + m) C_3 \Delta t^r$$

for all n and Δt with $mT \leq n\Delta t \leq (m+1)T$ and $0 \leq \Delta t \leq \Delta t_c$.

Since C_3 is independent of m, the Theorem implies that the error grows linearly with the number of periods that pass, and hence linearly with time.

Proof. The existence of B follows from Assumptions 1 and 2; without loss of generality, we take $B = B_1 \cup B_2$, the union of the two sets B given in those assumptions. Define

$$T^m z_0 = S(mT) z_0, \qquad T^m_{\Delta t} z_0 = S^{Nm}_{\Delta t} z_0, \qquad E^m z_0 = T^m_{\Delta t} z_0 - T^m z_0.$$

Thus,

$$\begin{aligned} \left\| E^{m+1} z_0 \right\| &= \left\| T^{(m+1)}_{\Delta t} z_0 - T^{(m+1)} z_0 \right\| \\ &= \left\| S^N_{\Delta t} S^{Nm}_{\Delta t} z_0 - S(T) S(mT) z_0 \right\| \\ &\leq \left\| S(T) S^{Nm}_{\Delta t} z_0 - S(T) S(mT) z_0 \right\| + \left\| S^N_{\Delta t} S^{Nm}_{\Delta t} z_0 - S(T) S^{Nm}_{\Delta t} z_0 \right\|. \end{aligned} \tag{2.3}$$

Note that $H(S_{\Delta t}^{Nm} z_0) = H(z_0)$ by Assumption 2; thus, we deduce that $S(T) S_{\Delta t}^{Nm} z_0 = S_{\Delta t}^{Nm} z_0$ by Assumption 1, since the period is uniquely determined by $H(z_0)$. Similarly $S(T)S(mT)z_0 = S(mT)z_0$. Thus,

$$\|E^m z_0\| = \|S_{\Delta t}^{Nm} z_0 - S(mT)z_0\| = \|S(T)S_{\Delta t}^{Nm} z_0 - S(T)S(mT)z_0\|. \tag{2.4}$$

By Assumption 2 with $\tilde{\Omega} = B$, $\tau = T$, and $n = N$,

$$\|S_{\Delta t}^{N} S_{\Delta t}^{Nm} z_0 - S(T) S_{\Delta t}^{Nm} z_0\| \le C_1(B, T)\Delta t^r \tag{2.5}$$

for $\Delta t \le \Delta t_c(B, T)$. Thus, (2.3)–(2.5) imply that

$$\|E^{m+1} z_0\| \le \|E^m z_0\| + C_1(B, T)\Delta t^r. \tag{2.6}$$

Since $E^0 z_0 = 0$, we have

$$\|E^m z_0\| \le mC_1(B, T)\Delta t^r. \tag{2.7}$$

This gives the desired result at times $t = mT$. It remains to fill in time nodes between integer multiples of the period T. Let $mT \le n\Delta t < (m+1)T$. We have for $n = mN + l$, with $0 \le l\Delta t < T$,

$$\begin{aligned} \|S_{\Delta t}^n z_0 - S(n\Delta t)z_0\| &= \|S_{\Delta t}^l S_{\Delta t}^{Nm} z_0 - S(l\Delta t)S(mT)z_0\| \\ &\le \|S(l\Delta t)S_{\Delta t}^{Nm} z_0 - S(l\Delta t)S(mT)z_0\| \\ &\quad + \|S(l\Delta t)S_{\Delta t}^{Nm} z_0 - S_{\Delta t}^l S_{\Delta t}^{Nm} z_0\|. \end{aligned} \tag{2.8}$$

Using (2.7) in (2.1) with $\tilde{\Omega} = B$, $z_1 = S(mT)z_0$, $z_2 = S_{\Delta t}^{Nm} z_0$, and $\delta = mC_1(B, T)\Delta t^r$, we obtain

$$\|S(l\Delta t)S_{\Delta t}^{Nm} z_0 - S(l\Delta t)S(mT)z_0\| \le C_2(B, T)mC_1(B, T)\Delta t^r, \tag{2.9}$$

since the true and numerical solutions both lie in B. Furthermore, Assumption 2 implies that

$$\|S(l\Delta t)S_{\Delta t}^{Nm} z_0 - S_{\Delta t}^l S_{\Delta t}^{Nm} z_0\| \le C_1(B, l\Delta t)\Delta t^r \le C_1(B, T)\Delta t^r, \tag{2.10}$$

for sufficiently small Δt depending only on B and T. Hence, (2.8)–(2.10) give

$$\|S_{\Delta t}^n z_0 - S(n\Delta t)z_0\| \le [1 + mC_2(B, T)]C_1(B, T)\Delta t^r$$

for all n and Δt with $mT \le n\Delta t \le (m+1)T$ and $0 \le \Delta t \le \Delta t_c(B, T)$. This gives the result with

$$C_3(B, T) = C_1(B, T) \max\{1, C_2(B, T)\}. \qquad \square$$

Important remarks

(i) The assumption that the true solution remains in a closed bounded subset of Ω for all $t \ge 0$ is a consequence of the conservation of the

Hamiltonian and the conservation of angular momentum in the example of Kepler's problem that motivates this work. In the next section, we analyse an approximation scheme that also conserves these two quantities so that the approximate solution also remains in a closed, bounded subset Ω for all $n \geq 0$. If, however, a scheme conserves only the Hamiltonian and not the angular momentum, then it is not possible to show on this basis alone that the numerical solution remains in a closed bounded subset of Ω for all $n \geq 0$. Nonetheless, a result similar to that proved here can be formulated except that Δt_c will depend upon m. The proof is straightforward and is left to the reader. An example of such a scheme is the continuous Galerkin method [4] and, in section 3, we present numerical results for this method also.

(ii) The key to the error analysis is to examine the error propagation over multiples of the period T as in [12]. It is also important that the propagation of errors be estimated in terms of the true solution operator, which has the property $S(T) \equiv I$ for all solutions on the same level set of H. See (2.3). Note that the standard way to analyse error propagation uses the numerical solution operator to propagate the errors to obtain

$$\begin{aligned} \left\| E^{m+1} z_0 \right\| \leq & \left\| S_{\Delta t}^N S_{\Delta t}^{Nm} z_0 - S_{\Delta t}^N S(mT) z_0 \right\| \\ & + \left\| S_{\Delta t}^N S(mT) z_0 - S(T) S(mT) z_0 \right\|, \end{aligned}$$

instead of the last line of (2.3). This, however, does not allow direct exploitation of the periodicity of solutions on the same level set of the Hamiltonian H. Convergence proofs exploiting the true solution operator for the error propagation may be found in [16], pages 491 and 492.

(iii) In the case where equation (1.1) is integrable, a result similar to the Theorem can be proved by different techniques which we now outline. In this case there is a locally invertible transformation $\Psi : z \in \mathbb{R}^{2N} \mapsto y = (\phi, a) \in \mathbb{R}^N \times \mathbb{R}^N$ under which (1.1) becomes

$$\begin{aligned} \phi_t &= \omega(a), \qquad \phi(0) = \phi_0, \\ a_t &= 0, \qquad a(0) = a_0; \end{aligned} \tag{2.11}$$

furthermore, the N integrals of the integrable system (1.1), denoted by $I(z) = (I_1(z), \ldots, I_N(z))^T \in \mathbb{R}^N$, satisfy $I(z) = a(0)$.

We apply a numerical method to (1.1) yielding the map (2.2). Employing the same change of variables Ψ as used for (1.1), we obtain the following approximation to (2.11) with local accuracy of $\mathcal{O}(\Delta t^{r+1})$:

$$\begin{aligned} \Phi_{n+1} &= \Phi_n + \Delta t \alpha(\Phi_n, A_n), \qquad \Phi_0 = \phi_0 \\ A_{n+1} &= A_n + \Delta t \beta(\Phi_n, A_n), \qquad A_0 = a_0. \end{aligned} \tag{2.12}$$

(To obtain this explicit form, we have inverted all nonlinear equations defining the implicit numerical method.) *Provided that the numerical method*

also conserves the same N integrals $I(\bullet)$ as the equation itself, it then follows that $\beta(\bullet, \bullet) \equiv 0$ so that

$$A_n = a_0 \qquad \forall n \geq 0,$$

or

$$\|A_n - a_n\| = 0 \qquad \forall n \geq 0.$$

Using consistency, we deduce that

$$\|\Phi_{n+1} - \phi((n+1)\Delta t)\| \leq \|\Phi_n - \phi(n\Delta t)\| + \mathcal{O}(\Delta t^{r+1})$$

yielding

$$\|\Phi_n - \phi(n\Delta t)\| \leq \mathcal{O}(T\Delta t^r)$$

for $0 \leq n\Delta t \leq T$, the required result. In [7], a more elaborate version of this technique is used to prove analogous results in a more complicated situation.

3. An example

In this section, we illustrate the theory in the previous section using Kepler's problem for two bodies. Let $u \in \mathbb{R}^2$ and $v \in \mathbb{R}^2$ solve

$$\begin{aligned} u_t &= v, & u(0) &= u_0, \\ v_t &= -\frac{u}{\|u\|} F'(\|u\|), & v(0) &= v_0, \end{aligned} \tag{3.1}$$

where $F(x) = -kx^{-1}$ for some real $k > 0$ and $\|\bullet\|$ denotes the Euclidean norm. Since $z^T = (u^T, v^T)$,

$$H(z) = \frac{1}{2}\|v\|^2 - k\|u\|^{-1}. \tag{3.2}$$

Thus, there exists $k_1 \in \mathbb{R}$ such that

$$H(z(t)) = -k_1, \qquad \forall t \geq 0. \tag{3.3}$$

It is well-known that all solutions are periodic if $k_1 > 0$, and that the period is uniquely determined by the energy ([1]). Furthermore, angular momentum is conserved. Since we are in two dimensions, this is equivalent to the statement that

$$v(t)^T J_1 u(t) = \alpha, \qquad \forall t \geq 0, \tag{3.4}$$

where α is a constant independent of t satisfying $|\alpha| = k_2$ for some $k_2 \geq 0$ and J_1 is a skew-symmetric matrix with norm 1. Thus (3.3) and (3.4) imply that

$$k_2 \leq \|v(t)\|\|u(t)\| = \|u(t)\|\sqrt{2[-k_1 + k/\|u(t)\|]}.$$

Therefore, there cannot be sequences $\{t_i\}$ such that $\|u(t_i)\| \to 0$ as $i \to \infty$. In fact, straightforward calculation shows that $2k_1k_2^2 \leq k^2$ and therefore that $u_- \leq \|u(t)\| \leq u_+$, where

$$u_\pm = \frac{k \pm \sqrt{[k^2 - 2k_1k_2^2]}}{2k_1}.$$

Then (3.3) implies that $v_- \leq \|v(t)\| \leq v_+$, where

$$v_\pm = \sqrt{2[k/u_\mp - k_1]}.$$

Thus Assumption 1 holds with

$$\Omega = \{z = (u^T, v^T)^T \in \mathbb{R}^4 : \|u\| > 0\}$$

and

$$B_1 = \{z = (u^T, v^T)^T \in \mathbb{R}^4 : u_- \leq \|u\| \leq u_+, v_- \leq \|v\| \leq v_+\}.$$

Now consider the following numerical approximation of (3.1) studied in [5]: given $(u_0^T, v_0^T)^T \in \mathbb{R}^4$, $\{u_n\}_{n=0}^\infty$ and $\{v_n\}_{n=0}^\infty$ satisfy

$$\begin{aligned} \frac{u_{n+1} - u_n}{\Delta t} &= \frac{v_{n+1} + v_n}{2}, \\ \frac{v_{n+1} - v_n}{\Delta t} &= -\frac{u_{n+1} + u_n}{\|u_{n+1}\| + \|u_n\|}\left[\frac{F(\|u_{n+1}\|) - F(\|u_n\|)}{\|u_{n+1}\| - \|u_n\|}\right]. \end{aligned} \tag{3.5}$$

This scheme conserves the Hamiltonian and also the angular momentum (see [5]). Thus, Assumption 2 holds with $B_2 = B_1$ where B_1 is given in Assumption 1; the convergence of the method is second order so that $r = 2$ and the constants C_1 and Δt_c depend only upon the time interval under consideration and the derivatives of H in a set determined by the initial data, using the positive invariance of B_1. Thus, the Theorem of section 2 shows that the error for this scheme grows at most linearly with time when $k_1 > 0$.

We present the results of a computation that confirms the analysis and shows that the linear-in-time bound on the error growth is sharp. We take the initial conditions $(0.4, 0, 0, 2)^T$ and compute to time 1300, which represents approximately 207 periods, with time step $\Delta t = \pi/500$. We compute the error every 0.5 time unit and plot the results in Fig. 1. In order to determine the rate of accumulation of error, we compute three lines fitted to subsets of the data using least squares. The first line is computed using all of the error data. The second line is computed using the minimum errors from each period. The third line is computed using the maximum errors from each period. The correlation for this last fit is 0.99999, which indicates

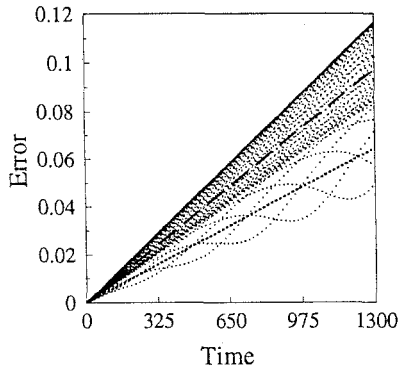

Figure 1
The error of the Gonzalez-Simo difference scheme computed with timestep $\Delta t = \pi/500$ starting with initial data (0.4, 0, 0, 2). The errors are plotted every 0.5 time unit.

that the maximum error grows linearly with the number of periods. Though the error varies greatly in each period, the overall trend is linear growth.

Note that for the total error in both position and velocity to grow linearly in time the velocity errors cannot have a consistent bias of one sign. This is illustrated in Fig. 2 in which the error growth for the velocities (third and fourth components of the solution) is shown. Whilst the envelope encompassing the errors grows linearly, the errors clearly oscillate around zero. We compute lines using the least squares fit, obtaining approximately lines with slope 8×10^{-8} for the third component and 2×10^{-7} for the fourth component, indicating that in an average sense, the errors in the velocity are accumulating extemely slowly.

To illustrate Important Remark (i) following the Theorem, we briefly describe computations with the continuous Galerkin ($q = 1$) finite element

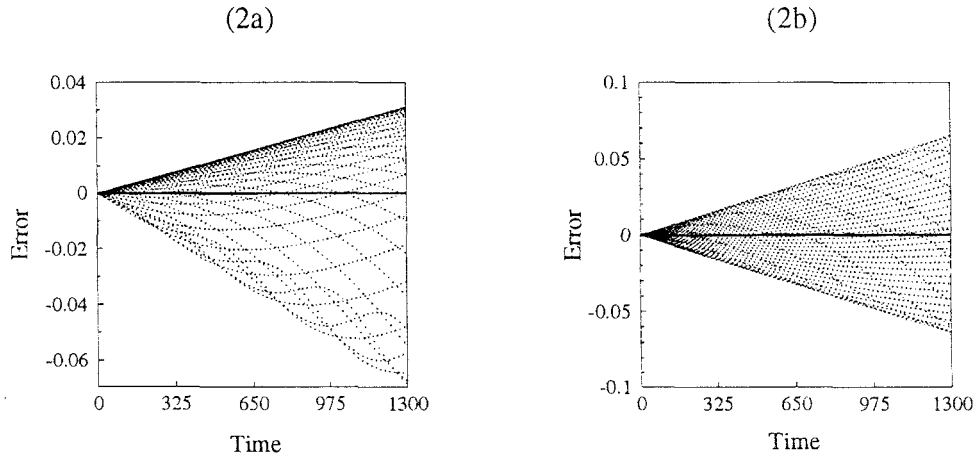

Figure 2
The error in the velocity components of the Gonzalez-Simo difference scheme computed with timestep $\Delta t = \pi/500$ starting with initial data (0.4, 0, 0, 2). The errors are plotted every 0.5 time unit.

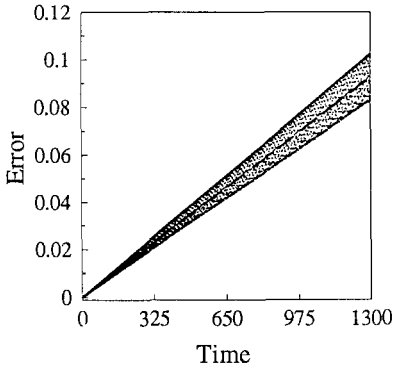

Figure 3
The error of the continuous Galerkin method computed with timestep $\Delta t = \pi/650$ starting with initial data (0.4, 0, 0, 2). The errors are plotted every 0.5 time unit.

method, which conserves the Hamiltonian but not the angular momentum. As remarked above, a result similar to the Theorem holds in this case but with Δt_c depending upon m. Let $t_n = n\Delta t$. This method produces a piecewise linear continuous approximation $Z(t)$ taking values Z_n at t_n. On the interval $[t_n, t_{n+1}]$,

$$Z(t) = Z_n \frac{t_{n+1} - t}{\Delta t} + Z_{n+1} \frac{t - t_n}{\Delta t}, \tag{3.6}$$

where the new nodal value Z_{n+1} satisfies

$$Z_{n+1} = Z_n + \int_{t_n}^{t_{n+1}} J\nabla H(Z(t))\, dt. \tag{3.7}$$

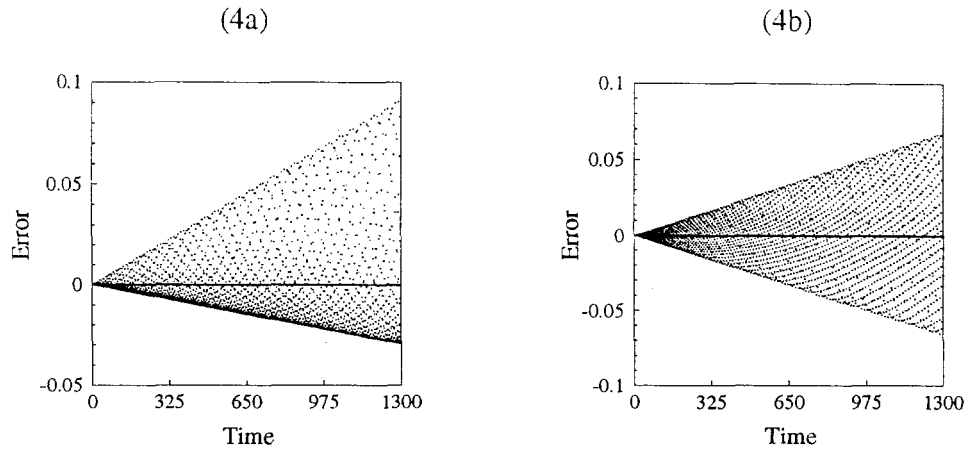

Figure 4
The error in the velocity components of the continuous Galerkin method computed with timestep $\Delta t = \pi/650$ starting with initial data (0.4, 0, 0, 2). The errors are plotted every 0.5 time unit.

This defines a nonlinear equation for Z_{n+1} by substitution of the expression (3.6) for $Z(t)$ on $[t_n, t_{n+1}]$. It may be shown that the continuous Galerkin method conserves the Hamiltonian by taking the inner product of (3.7) with $J\dot{Z}_n$, where $\dot{Z}_n$ denotes the derivative of Z on the time interval $[t_n, t_{n+1}]$; see [4].

We compute again using initial condition $(0.4, 0, 0, 2)^T$ to time 1300, but we use timestep $\Delta t = \pi/650$ so that the error of this approximation is roughly equal to the error of the Gonzalez-Simo scheme. (Computations for the continuous Galerkin method with $\Delta t = \pi/500$ have the same qualitative behavior.) In Fig. 3, we plot the error recorded every 0.5 time unit with three least square line fits computed using all of the data, the minimum errors in each period, and the maximum errors in each period, respectively. Again the correlations are very close to 1 and verify that the error grows linearly. In Fig. 4, we plot the errors in the velocity components together with least square line fits. These lines have slopes -1.58×10^{-7} and -9.41×10^{-8} respectively, indicating that in an average sense, the errors in the velocity are accumulating extremely slowly.

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References

[1] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, New York 1989.
[2] J. Baumgarte and E. Stiefel, *Stabilization by manipulation of the Hamiltonian*, Cel. Mech. *10*, 71–83 (1974).
[3] J. de Frutos and J. M. Sanz-Serna, *Erring and being conservative*. In *Numerical Analysis*, D. F. Griffiths and G. A. Watson (eds.), Pitman 1994.
[4] D. Estep and D. French, *Global error control for the continuous Galerkin finite element method for ordinary differential equations*, RAIRO Modélisation Mathématique et Analyse Numérique *28*, 815–852 (1994).
[5] O. Gonzalez and J. C. Simo, *On the stability of symplectic and energy-momentum algorithms for nonlinear Hamiltonian systems with symmetry*, Submitted to Comp. Meth. Appl. Mech. Eng. (1994).
[6] W. B. Gordon, *On the relation between period and energy in periodic dynamical systems*. J. Appl. Math. and Mech. *19*, 111–114 (1969).
[7] U. Kirchgraber, *On the Stiefel-Baumgarte stabilization procedure*, J. Appl. Math. and Physics *30*, 272–291 (1979).
[8] D. Okunbor, *Variable step size does not harm second-order integrators for Hamiltonian systems*, J. Comp. Appl. Math. *47*, 273–279 (1993).
[9] J. M. Sanz-Serna, *Symplectic integrators for Hamiltonian problems: an overview*. Acta Numerica 1992, Cambridgge University Press.

[10] J. M. Sanz-Serna, *Two topics in nonlinear stability*. In *Advances in Numerical Analysis, Volume I*, W. Light (ed.), Oxford University Press 1992.
[11] J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, 1994.
[12] J. M. Sanz-Serna and M. P. Calvo, *The development of variable-step symplectic integrators, with application to the two-body problem*, SIAM J. Sci. Stat. Comp. *14*, 936–952 (1993).
[13] J. C. Simo, N. Tarnow and K. K. Wong, *Exact energy-mommentum conserving algorithms and symplectic schemes for nonlinear dynamics*, Comp. Meth. Appl. Mech. Eng. *1*, 63–116 (1992).
[14] J. C. Simo and N. Tarnow, *The discrete energy-momentum method. Conserving algorithms for nonlinear elastodynamics*, ZAMP *43*, 757–793 (1992).
[15] E. Stiefel and G. Scheifele, *Linear and Regular Celestial Mechanics*, Springer, New York 1971.
[16] A. M. Stuart, *Numerical Analysis of Dynamical Systems*. Appears in Acta Numerica 1994, Cambridge University Press, Cambridge 1994.
[17] H. Yoshida, *Recent progress in the theory and application of symplectic integrators*, Cel. Mech. Dyn. Atsr. *56*, 27–43 (1993).
[18] G. Zhong and J. E. Marsden, *Lie-Poisson Hamilton-Jacobi theory and Lie-Poisson integrators*, Phys. Lett. A *133*, 134–139 (1988).

Abstract

In this note, we consider numerical methods for a class of Hamiltonian systems that preserve the Hamiltonian. We show that the rate of growth of error is at most linear in time when such methods are applied to problems with period uniquely determined by the value of the Hamiltonian. This contrasts to generic numerical schemes, for which the rate of error growth is superlinear. Asymptotically, the rate of error growth for symplectic schemes is also linear. Hence, Hamiltonian-conserving schemes are competitive with symplectic schemes in this respect. The theory is illustrated with a computation performed on Kepler's problem for the interaction of two bodies.

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