Energy conservation with non-symplectic methods: examples and counter-examples

Faou, Erwan; Hairer, Ernst; Pham, Truong-Linh

How to cite

FAOU, Erwan, HAIRER, Ernst, PHAM, Truong-Linh. Energy conservation with non-symplectic methods: examples and counter-examples. In: BIT, 2004, vol. 44, n° 4, p. 699–709. doi: 10.1007/s10543-004-5240-6

This publication URL: https://archive-ouverte.unige.ch/unige:12121
Publication DOI: 10.1007/s10543-004-5240-6

ENERGY CONSERVATION WITH NON-SYMPLECTIC METHODS: EXAMPLES AND COUNTER-EXAMPLES

ERWAN FAOU[1], ERNST HAIRER[2] and TRUONG-LINH PHAM[2]

[1] *INRIA Rennes, Campus Beaulieu, F-35042 Rennes Cedex, France.*
email: Erwan.Faou@irisa.fr

[2] *Section de Mathématiques, Univ. de Genève, CH-1211 Genève 24, Switzerland.*
email: Ernst.Hairer@math.unige.ch, Truong-Linh.Pham@math.unige.ch

Abstract.

Energy conservation of numerical integrators is well understood for symplectic one-step methods. This article provides new insight into energy conservation with non-symplectic methods. Sufficient conditions and counter-examples are presented.

AMS subject classification: 65L06, 65P10, 37J99

Key words: Hamiltonian systems, energy conservation, backward error analysis, symmetric and symplectic methods.

1 Introduction.

Our interest is the numerical solution of Hamiltonian systems

$$\begin{aligned} \dot p &= -\nabla_q H(p,q) \\ \dot q &= \nabla_p H(p,q) \end{aligned} \qquad \text{or} \qquad \dot y = J^{-1}\nabla H(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{1.1}$$

where $y = (p,q)^T$ and $H(y) = H(p,q)$ is a real-valued smooth function. Since J is skew-symmetric, the Hamiltonian $H(y)$ is a first integral of the system which means that it is constant along exact solutions of (1.1). In applications, $H(y)$ is often the total energy (sum of kinetic and potential energy of a mechanical system) so that this property is equivalent to energy conservation.

For a numerical integration it is of interest to know whether the Hamiltonian remains also constant or nearly constant along the numerical solution over very long time intervals. It is known that

- symplectic one-step methods nearly conserve the Hamiltonian of an arbitray system (1.1) over exponentially long times; [1] and [4],
- symmetric reversible one-step methods nearly conserve all action variables of a reversible integrable system; see chapter XI of [6],
- certain symmetric multistep methods nearly conserve the Hamiltonian of systems, where $H(p,q) = \frac{1}{2}p^Tp + U(q)$; see [5].

In many other situations it is observed that the numerical solution also well conserves the Hamiltonian over long times but a theoretical explanation is missing.

The aim of this paper is to study the energy conservation of a wide class of numerical integrators including Runge-Kutta methods, Hermite-Obreschkoff methods, the underlying one-step method of multistep and general linear methods. We give conditions on the coefficients of the method that guarantee the existence of a first integral of the modified equation that is close to the Hamiltonian (Section 3). This then implies energy conservation. We further present counter-examples (Section 4) showing that not all symmetric Runge-Kutta methods conserve the Hamiltonian even if (1.1) is reversible with respect to the reflection $p \leftrightarrow -p$.

2 B-series and backward error analysis.

For the numerical treatment of differential equations

$$\dot{y} = f(y), \tag{2.1}$$

we consider numerical methods $y_{n+1} = \Phi_h(y_n)$ whose Taylor series around $h = 0$ has the form of a B-series. Based on the seminal work of Butcher [2], such series have been introduced and studied in [8]. A complete and comprehensive presentation is given in Chapter III of [6]. We shall closely follow the notation used in this monograph.

Let T be the set of trees. We use the notation $\tau = [\tau_1, \dots, \tau_m]$ for the tree which is obtained from $\tau_1, \dots, \tau_m$ by grafting their roots to a new vertex which then becomes the root of the tree τ. The number of vertices is denoted by $|\tau|$, and the *symmetry coefficient* is defined recursively by

$$\sigma(\bullet) = 1, \qquad \sigma(\tau) = \sigma(\tau_1) \cdot \ldots \cdot \sigma(\tau_m) \cdot \mu_1! \, \mu_2! \cdot \ldots \tag{2.2}$$

where the integers $\mu_1, \mu_2, \dots$ count equal trees among $\tau_1, \dots, \tau_m$. The so-called *elementary differentials* $F(\tau)(y)$ are given by

$$F(\bullet)(y) = f(y), \qquad F(\tau)(y) = f^{(m)}(y)\big(F(\tau_1)(y), \dots, F(\tau_m)(y)\big). \tag{2.3}$$

For real coefficients $a(\emptyset)$ and $a(\tau)$ for $\tau \in T$, a series of the form

$$B(a, y) = a(\emptyset) y + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} \, a(\tau) \, F(\tau)(y) \tag{2.4}$$

is called a *B-series*. Not only Runge-Kutta methods can be written in the form $y_{n+1} = B(a, y_n)$, but also multi-stage multi-derivative one-step methods and the underlying one-step method of multistep and general linear methods.

Backward error analysis is the main tool for getting insight into the long-time behaviour of numerical integrators. It is based on the observation that the numerical solution of a one-step method $y_{n+1} = \Phi_h(y_n)$ can be (formally)

interpreted as the exact solution of a *modified differential equation*. As proved in [3] (see also Section IX.9 of [6]) this modified equation is given by

$$\dot{y} = \sum_{\tau \in T} \frac{h^{|\tau|-1}}{\sigma(\tau)}\, b(\tau)\, F(\tau)(y), \tag{2.5}$$

or equivalently, $h\dot{y} = B(b, y)$ with coefficients $b(\emptyset) = 0$ and $b(\tau)$ that are in a one-to-one correspondence with the coefficients $a(\tau)$ of the B-series for $\Phi_h(y)$.

3 First integrals composed of elementary Hamiltonians.

The modified differential equation of a symplectic method applied to a Hamiltonian system (1.1) is again Hamiltonian. It has been observed in [3] that the Hamiltonian of the modified equation has a very special structure: it is a linear combination of so-called elementary Hamiltonians. Such expressions have first been considered in [10] (called canonical elementary differentials) for the study of order conditions of symplectic Runge-Kutta schemes.

Elementary Hamiltonians are defined by

$$H(\bullet)(y) = H(y), \qquad H(\tau)(y) = H^{(m)}(y)\big(F(\tau_1)(y), \ldots, F(\tau_m)(y)\big), \tag{3.1}$$

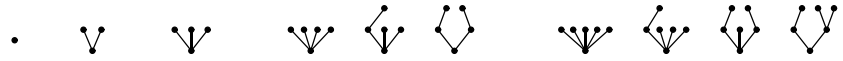
where $F(\tau_i)(y)$ are elementary differentials corresponding to $f(y) = J^{-1}\nabla H(y)$. Denoting, for $u = [u_1, \ldots, u_m] \in T$ and $v \in T$, by $u \circ v = [u_1, \ldots, u_m, v]$ the *Butcher product* of two trees, one verifies without difficulty (Lemma 7.2 of [10] or Section IX.10.1 of [6]) that

$$H(u \circ v)(y) = -H(v \circ u)(y) \qquad \text{and} \qquad H(u \circ u)(y) = 0.$$

This suggests to consider the equivalence relation $u \circ v \sim v \circ u$ on T. For two trees τ, θ of the same equivalence class we let $\kappa(\tau, \theta)$ be the number of root changes ($u \circ v \leftrightarrow v \circ u$) that are necessary to obtain θ from τ. From every equivalence class that does not contain a tree of the form $u \circ u$ (superfluous tree) we then select one tree and we collect these trees in the set T^*. The numbers of trees in T^* having k vertices is given in the following table:

k	1	2	3	4	5	6	7	8
	1	0	1	1	3	4	11	25

A possible choice for the trees in T^* with not more than 6 vertices is as follows:



We recall that for symplectic methods the modified differential equation (2.5) is Hamiltonian (see [3]) with a function of the form

$$H(c, y) = \sum_{\tau \in T^*} \frac{h^{|\tau|-1}}{\sigma(\tau)}\, c(\tau)\, H(\tau)(y) \tag{3.2}$$

with real coefficients $c(\tau)$. This motivates to study whether a function of the form (3.2) can be a first integral of (2.5) also if the corresponding method is not symplectic.

LEMMA 3.1. *Let $y(t)$ be a solution of the differential equation (2.5), i.e. $h\dot{y}(t) = B(b, y(t))$. We then have*

$$\frac{d}{dt} H\big(c, y(t)\big) = H\big(\delta_b c, y(t)\big)$$

where, for $\tau \in T^*$,

$$\delta_b c(\tau) = \sum_{\theta \sim \tau} (-1)^{\kappa(\tau,\theta)} \, \frac{\sigma(\tau)}{\sigma(\theta)} \sum_{\omega \in T^* \cap SP(\theta)} c(\omega)\, b(\theta \setminus \omega). \tag{3.3}$$

The first sum is over all trees θ that are equivalent to τ, and the second sum is over all splittings of θ; a splitting is obtained by removing one branch of θ which gives rise to two trees: δ has the same root as the former θ, and the root of $\theta \setminus \delta$ is the vertex connected with the removed branch.

PROOF. The proof is nearly identical to that of Lemma IX.9.1 in [6] and therefore omitted. □

COROLLARY 3.2. *The function $H(c, y)$ of (3.2) is a first integral of the differential equation (2.5) for every $H(y)$ if and only if*

$$\delta_b c(\tau) = 0 \quad \text{for all } \tau \in T^*. \tag{3.4}$$

PROOF. The sufficiency follows from Lemma 3.1 and the necessity is a consequence of the independence of the elementary Hamiltonians. In fact, with the techniques of the proof of [6, Theorem VI.7.1] one can show that for every tree $\tau \in T^*$ there exists a polynomial Hamiltonian such that the first component of $F(\tau)(0)$ vanishes for all trees except for τ. □

COROLLARY 3.3. *Let $b(\tau)$ be the coefficients (2.5) corresponding to a symmetric method, i.e., $b(\tau) = 0$ for trees with an even number of vertices. Then, the condition*

$$\delta_b c(\tau) = 0 \quad \text{for } \tau \in T^* \text{ with odd } |\tau| \tag{3.5}$$

can be satisfied by putting $c(\tau) = 0$ for trees with even $|\tau|$.

PROOF. If τ has an odd number of vertices, then either θ or ω of formula (3.3) has an even number of vertices. □

For $\tau = \bullet$ there is no splitting and the condition (3.4) is trivially fulfilled. There is no tree in T^* with two vertices. For the next trees of T^* with no more than six vertices, the expressions for $\delta_b c(\tau)$ are given in Table 3.1.

Solving the system (3.4). We consider a consistent method, i.e., $b(\bullet) = 1$, and we search for a first integral $H(c, y)$ close to the Hamiltonian, i.e., $c(\bullet) = 1$.

$|\tau| = 3$: The condition (3.4) for $\tau =$ then implies $b($  $) = 0$, which means that the method has to be of order two.

$|\tau| = 4$: There is only one tree in T^* with four vertices. The corresponding condition can be satisfied by choosing $c($  $) = b($ $)$.

Table 3.1: Formulas for $\delta_b c(\tau)$ for trees $\tau \in T^*$.

$$
\begin{aligned}
\delta_b c(\tau_1) &= -2\, c(\bullet) b(\tau_2) \\
\delta_b c(\tau_2) &= 3\, c(\tau_1) b(\bullet) - 3\, c(\bullet) b(\tau_1) \\
\delta_b c(\tau_3) &= 4\, c(\tau_2) b(\bullet) - 4\, c(\bullet) b(\tau_2) \\
\delta_b c(\tau_4) &= c(\tau_2) b(\bullet) + c(\tau_1) b(\tau_2) + c(\bullet) b(\tau_5) - 2\, c(\bullet) b(\tau_4) \\
\delta_b c(\tau_6) &= 2\, c(\bullet) b(\tau_7) - 2\, c(\tau_1) b(\tau_2) \\
\delta_b c(\tau_8) &= 5\, c(\tau_3) b(\bullet) - 5\, c(\bullet) b(\tau_3) \\
\delta_b c(\tau_9) &= 3\, c(\tau_4) b(\bullet) + c(\tau_8) b(\bullet) + c(\tau_2) b(\tau_2) \\
&\quad -3\, c(\bullet) b(\tau_4) + c(\bullet) b(\tau_5) \\
\delta_b c(\tau_{10}) &= 2\, c(\tau_4) b(\bullet) + c(\tau_6) b(\bullet) - c(\bullet) b(\tau_6) + 2\, c(\bullet) b(\tau_9) \\
\delta_b c(\tau_{11}) &= 2c(\tau_6) b(\bullet) - c(\tau_4) b(\bullet) - c(\tau_2) b(\tau_2) - c(\tau_1) b(\tau_1) \\
&\quad -c(\tau_1) b(\tau_7) + 2\, c(\bullet) b(\tau_{10}) + c(\bullet) b(\tau_{11})
\end{aligned}
$$

$|\tau| = 5$: The third condition yields $b([[[\bullet]]]) = 0$. Choosing $c(\tau_5)$ such that one of the other two conditions holds, we still have to satisfy

$$b(\tau_5) + b(\tau_9) - 2\, b(\tau_{10}) = 0. \tag{3.6}$$

This condition is satisfied for symplectic methods, for which $b(u \circ v) + b(v \circ u) = 0$, and also for symmetric methods, for which $b(\tau) = 0$ for trees with an even number of vertices.

$|\tau| = 6$: There are four conditions for three $c(\tau)$ coefficients. Assuming (3.4) for trees with less than five vertices, these four conditions admit a solution if and only if

$$
\begin{aligned}
&5\, b(\tau_{12}) + 5\, b(\tau_9) + 6\, b(\tau_{11}) + 6\, b(\tau_{10}) - 12\, b(\tau_9) + 3\, b(\tau_{13}) \\
&\qquad -15\, b(\tau_{14}) - 3\, b(\tau_1)\Big(b(\tau_3) + b(\tau_7)\Big) = 0.
\end{aligned} \tag{3.7}
$$

This relation is obviously satisfied by every symplectic method. However, as we shall see soon, there are symmetric methods that do not satisfy (3.7).

Discussion of the condition (3.7). For various symmetric methods of order 4 (i.e., $b(\tau) = 0$ for $1 < |\tau| < 5$) we compute the coefficients $b(\tau)$ of the leading perturbation term in (2.5) and also the expression (3.7). They are listed in Table 3.2. None of the considered methods is symplectic.

Table 3.2: Coefficients $b(\tau)$ and expression (3.7) for methods of order 4.

method								(3.7)
Lobatto IIIA	$\frac{1}{120}$	$\frac{1}{240}$	$\frac{1}{480}$	$-\frac{1}{120}$	$-\frac{1}{240}$	$\frac{1}{720}$	$-\frac{1}{360}$	0
Lobatto IIIB	$\frac{1}{120}$	$-\frac{1}{360}$	$-\frac{1}{720}$	$-\frac{1}{120}$	$\frac{1}{360}$	$\frac{1}{720}$	$\frac{1}{240}$	$\frac{1}{48}$
Hermite-Obresch.	$-\frac{1}{30}$	$-\frac{1}{60}$	$-\frac{1}{120}$	$-\frac{1}{120}$	$-\frac{1}{240}$	$-\frac{1}{180}$	$-\frac{1}{360}$	0
multistep	$\frac{C}{5}$	$\frac{C}{10}$	$\frac{C}{20}$	$\frac{C}{20}$	$\frac{C}{40}$	$\frac{C}{30}$	$\frac{C}{60}$	0

Surprisingly, the 3-stage collocation method Lobatto IIIA (see [6, page 31] for the coefficients) satisfies the condition (3.7). This implies for every Hamiltonian system (reversible or not reversible) that the dominating error term in the numerical Hamiltonian does not have any drift.

For the underlying one-step method of multistep methods, not only the condition (3.7) is satisfied, but there exists a modified Hamiltonian (3.2) such that (3.4) is satisfied for all trees. This statement can be obtained similar to that of Proposition 1 in [5]. Due to uncontrolled parasitic solutions of non-partitioned multistep methods for first order differential equations, this property is however of little value. The leading error term for Hermite-Obreschkoff methods ([7, page 277]) is the same as for multistep methods.

The 3-stage Lobatto IIIB method (see [6, page 33]) does not satisfy the condition (3.7). We therefore expect a drift in the numerical Hamiltonian.

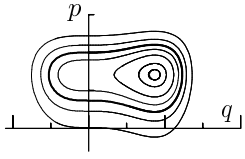
4 Examples for energy drift with symmetric methods.

This section is devoted to numerical experiments confirming the previous theoretical investigations. In particular, we present examples of reversible systems where symmetric methods produce an energy drift.

4.1 Problems with one degree of freedom

Hamiltonian systems (1.1) with scalar p and q are easy to understand. We let

$$\begin{aligned} H(p,q) &= T(p)+U(q), \\ T(p) &= \frac{p^3}{3}-\frac{p}{2}, \\ U(q) &= \frac{q^6}{30}+\frac{q^4}{4}-\frac{q^3}{3}+\frac{1}{6}. \end{aligned} \tag{4.1}$$



The Hamiltonian is not an even function in p and therefore it does not lead to a reversible system. This is also seen from its level sets. We apply both, the Lobatto IIIA and the Lobatto IIIB method, to this Hamiltonian system with initial values $p(0)=1$ and $q(0)=0$ so that the solution is periodic and

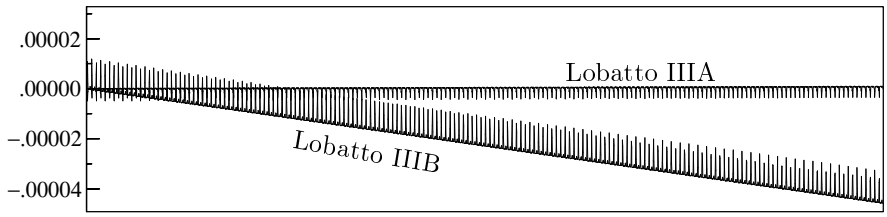


Figure 4.1: Numerical Hamiltonian of Lobatto methods for the problem (4.1); step size $h = 0.16$, integration interval $[0, 1600]$.

$p(t)$ remains positive for all times. For the integration interval $[0, 1600]$ and step size $h = 0.16$ the result is shown in Figure 4.1. Repeating the experiment with different step sizes and on longer time intervals, one finds that the error in the Hamiltonian behaves like $\mathcal{O}(th^4)$ for the Lobatto IIIB method, and like $\mathcal{O}(h^4 + th^6)$ for the Lobatto IIIA method. The presence of the $\mathcal{O}(th^6)$ term indicates that we cannot expect the 3-stage Lobatto IIIA method to satisfy the condition (3.4) for trees with eight vertices.

With the functions $T(p)$ and $U(q)$ of (4.1) we next consider the Hamiltonian system with

$$H(p,q) = \big(T(p) + U(q)\big)\big(T(-p) + U(q)\big), \tag{4.2}$$

which is reversible, i.e., it satisfies $H(-p,q) = H(p,q)$. Due to the fact that $T(-p) = -T(p)$, it is also separable. Moreover, since the initial values were chosen such that $H\big(p(0), q(0)\big) = 0$, the curve $H(p,q) = 0$ is the same for both Hamiltonians. We therefore expect a similar behaviour for the numerical solution. This is indeed the case as can be observed in Figure 4.2 (notice that the errors are smaller by a factor of about ten).

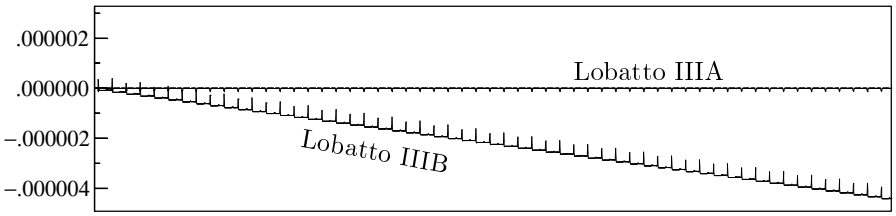


Figure 4.2: Numerical Hamiltonian of Lobatto methods for the problem (4.2); step size $h = 0.16$, integration interval $[0, 1600]$.

4.2 Problem with one degree of freedom on a cylinder

Another simple example is the perturbed pendulum equation

$$H(p,q) = \tfrac{1}{2}\, p^2 - \cos q + \tfrac{1}{5}\, \sin(2q). \tag{4.3}$$

If we consider initial values $p(0) = 2.5$, $q(0) = 0$ with sufficiently large initial velocity, $p(t)$ stays positive for all times and the symmetry $p \leftrightarrow -p$ does not affect the numerical solution. Notice that $q(t)$ increases without bound, but the potential is 2π-periodic which implies that the solution stays on a closed curve of the cylinder $\mathbb{R} \times S^1$. The perturbation term in the potential destroys the symmetry in q.

The numerical solution has the same behaviour as in the previous examples. There is an energy drift of size $\mathcal{O}(th^4)$ for the Lobatto IIIB method and the dominating error term in the Hamiltonian is bounded for the Lobatto IIIA method. Without the term $\sin(2q)$ in (4.3) all symmetric one-step methods nearly conserve the Hamiltonian.

4.3 Polynomial Hamiltonians of degree at most four

For Hamiltonians $H(y)$ that are polynomials of degree at most four, the elementary Hamiltonian corresponding to the tree  vanishes identically. Therefore, the condition (3.4) need not be considered for this tree, and the remaining three conditions can always be satisfied by the three $c(\tau)$ coefficients. This implies that, for example for the Hénon–Heiles Hamiltonian

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}\big(p_1^2 + p_2^2\big) + \frac{1}{2}\big(q_1^2 + q_2^2\big) + q_1 q_2^2 - \frac{1}{3}\, q_1^3, \tag{4.4}$$

the leading error term in the numerical Hamiltonian remains bounded by all methods of order four. Numerical experiments indicate that in this case also higher order error terms are bounded by symmetric methods such as Lobatto IIIB, even if the initial values are chosen so that the solutions are chaotic. This observation is still without a theoretical explanation.

4.4 Mechanical systems with two degrees of freedom

We finally consider the two degrees of freedom Hamiltonian

$$H(p, q) = \frac{1}{2}\, p^T p + \frac{\omega^2}{2}\big(\|q\| - 1\big)^2 + q_2 - \frac{1}{\|q - a\|}. \tag{4.5}$$

This is a model of a spring pendulum with exterior forces. The spring is modelled by a harmonic potential with frequency $\omega = 2$ (Hooke's law). The exterior forces are gravitation and attraction to a mass point situated at $a = (-3, -5)^T$. The initial values for the position of the free mass point are $q(0) = (0, 1)^T$ (upright position), and for the velocity $p(0) = (-1, -0.5)^T$. The pendulum thus turns around the fixed end of the spring which is at the origin. The two exterior potentials are chosen so that no symmetry in the q-variables is present.

The Hamiltonian along the numerical solution obtained by different methods and step size $h = 0.1$ is shown in Figure 4.3. For the Lobatto IIIB method one clearly observes a drift and, repeating the experiment with halved step sizes, one finds that the error in the Hamiltonian behaves like $\mathcal{O}(th^4)$. For the Lobatto IIIA method one observes a $\mathcal{O}(h^4)$ error behaviour on this relatively short time interval. To get more insight into the behaviour of this method,

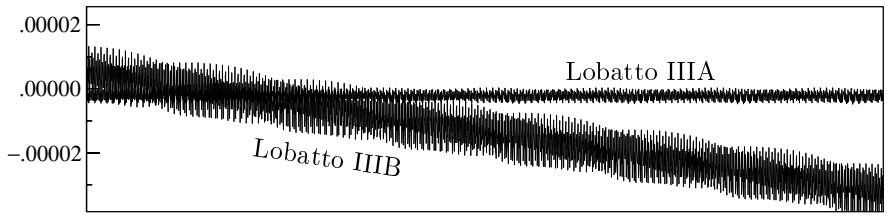


Figure 4.3: Numerical Hamiltonian of Lobatto methods for the spring pendulum (4.5); step size $h = 0.1$, integration interval $[0, 3000]$.

we apply it on a much longer time interval $[0, 150\,000]$ with two different step sizes $h = 0.1$ and $h = 0.1 \cdot 2^{1/6}$. To diminish the $\mathcal{O}(h^4)$ oscillations, we plot in Figure 4.4 the error of the mean of 250 consecutive values of $H(p_n, q_n)$ as a function of time. On a finer scale a drift becomes visible with a slope that is twice as large for the larger step size. This shows that the slope is proportional to h^6, so that the overall behaviour of the energy error of the Lobatto IIIA method is $\mathcal{O}(h^4 + th^6)$. This again confirms the theoretical investigations of the previous section. Removing one of the exterior forces (gravitation or attraction to a), the error in the Hamiltonian remains bounded of size $\mathcal{O}(h^4)$ without any drift (even not in higher order terms) for both Lobatto methods.

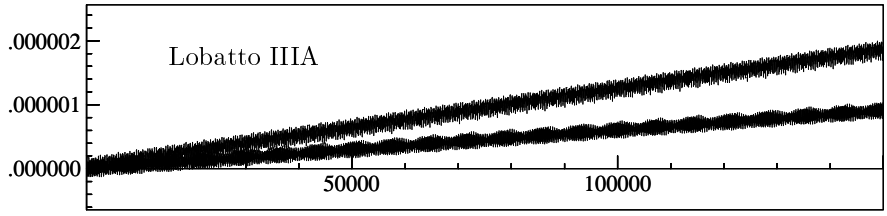


Figure 4.4: Numerical Hamiltonian of Lobatto methods for the spring pendulum (4.5); step sizes $h = 0.1$ and $h = 0.1 \cdot 2^{1/6}$, integration interval $[0, 150\,000]$.

5 Conclusion and comments

A Hamiltonian system is reversible with respect to the reflection $(p, q) \leftrightarrow (-p, q)$ if the Hamiltonian is an even function of p, i.e.,

$$H(-p, q) = H(p, q). \tag{5.1}$$

It is generally believed that symmetric methods applied to reversible Hamiltonian systems nearly preserve the energy over long times. The Hamiltonians (4.2), (4.3), and (4.5), combined with the 3-stage Lobatto IIIB method provide counter-examples to this belief.

In all our experiments, the reversible Hamiltonians and the initial values are chosen such that the trajectories $\big(p(t), q(t)\big)$ and $\big(-p(-t), q(-t)\big)$, which both

satisfy the same differential equation, are well separated. To prove near energy conservation for symmetric methods applied to reversible Hamiltonian systems, such situations have to be excluded. Certain ergodicity assumptions on the trajectory (probably difficult to verify) seem to be necessary. We refer to [9] and [11] for the study of related questions.

For the problems (4.3) and (4.5), s-stable symmetric multistep methods for second order differential equations perform qualitatively better (see [5]) than symmetric one-step methods violating (3.4), such as the 3-stage Lobatto IIIB method.

The investigations of this article can be extended straightforwardly to *partitioned methods* that can be expressed as P-series (i.e., the p and q variables in (1.1) are treated by different discretizations, see [6, Section III.2]). In this case, the elementary Hamiltonians (3.1) have to be replaced by those of [6, Definition IX.10.4], and the extension of Lemma 3.1 will be based on [6, Lemma IX.9.3]. Since the number of bi-coloured trees is larger, one has more coefficients available in (3.2), but the number of conditions in (3.4) increases accordingly.

Acknowledgement.

The authors are grateful to Christian Lubich and Gerhard Wanner for their interest in this work and for their useful comments on earlier versions.

REFERENCES

1. G. Benettin and A. Giorgilli. On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms. *J. Statist. Phys.*, 74:1117–1143, 1994.
2. J. C. Butcher. An algebraic theory of integration methods. *Math. Comput.*, 26:79–106, 1972.
3. E. Hairer. Backward analysis of numerical integrators and symplectic methods. *Annals of Numerical Mathematics*, 1:107–132, 1994.
4. E. Hairer and C. Lubich. The life-span of backward error analysis for numerical integrators. *Numer. Math.*, 76:441–462, 1997. Erratum: http://www.unige.ch/math/folks/hairer/.
5. E. Hairer and C. Lubich. Symmetric multistep methods over long times. *Numer. Math.*, 97:699–723, 2004.
6. E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics 31. Springer, Berlin, 2002.
7. E. Hairer, S. P. Nørsett, and G. Wanner. *Solving Ordinary Differential Equations I. Nonstiff Problems*. Springer Series in Computational Mathematics 8. Springer, Berlin, 2 edition, 1993.
8. E. Hairer and G. Wanner. On the Butcher group and general multi-value methods. *Computing*, 13:1–15, 1974.

9. R. I. McLachlan and M. Perlmutter. Energy drift in reversible time integration. *Preprint*, 2003.
10. J. M. Sanz-Serna and L. Abia. Order conditions for canonical Runge-Kutta schemes. *SIAM J. Numer. Anal.*, 28:1081–1096, 1991.
11. P. F. Tupper. Ergodicity and numerical simulation. *Preprint*, 2003.