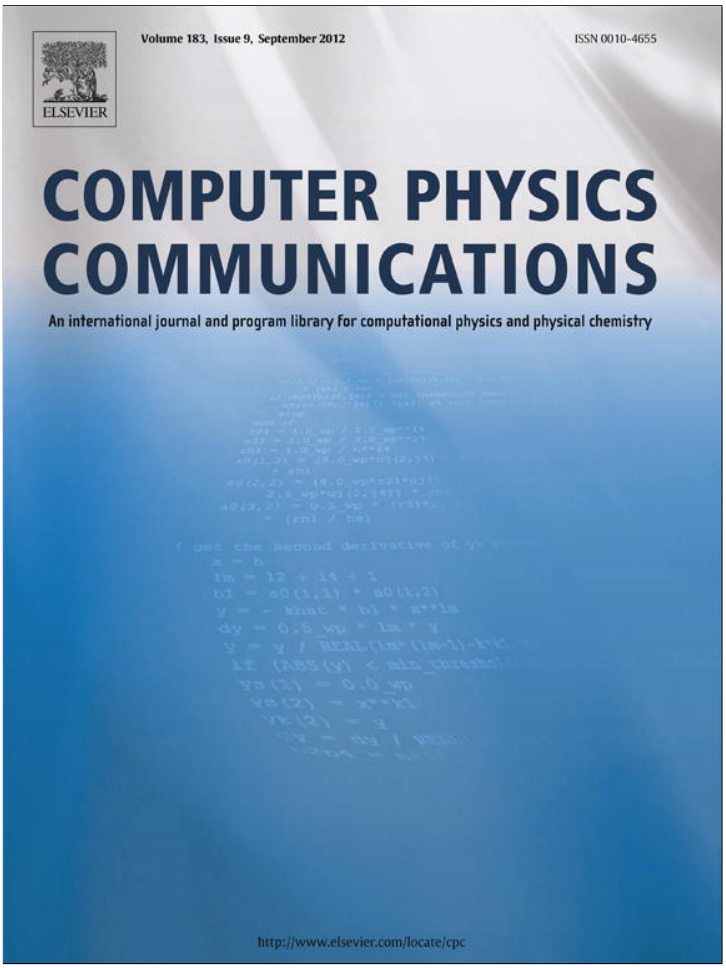

Computer Physics Communications 183 (2012) 1860–1868

Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

A two-step, fourth-order method with energy preserving properties☆

Luigi Brugnano [a], Felice Iavernaro [b,*], Donato Trigiante [1]

[a] Dipartimento di Matematica "U. Dini", Università di Firenze, Italy
[b] Dipartimento di Matematica, Università di Bari, Italy

ARTICLE INFO

Article history:
Received 3 June 2011
Received in revised form
5 April 2012
Accepted 10 April 2012
Available online 25 April 2012

Keywords:
Ordinary differential equations
Mono-implicit methods
Multistep methods
One-leg methods
Canonical Hamiltonian problems
Hamiltonian boundary value methods
Energy preserving methods
Energy drift

ABSTRACT

We introduce a family of fourth-order two-step methods that preserve the energy function of canonical polynomial Hamiltonian systems. As is the case with linear mutistep and one-leg methods, a prerogative of the new formulae is that the associated nonlinear systems to be solved at each step of the integration procedure have the very same dimension of the underlying continuous problem.

The key tools in the new methods are the line integral associated with a conservative vector field (such as the one defined by a Hamiltonian dynamical system) and its discretization obtained by the aid of a quadrature formula. Energy conservation is equivalent to the requirement that the quadrature is exact, which turns out to be always the case in the event that the Hamiltonian function is a polynomial and the degree of precision of the quadrature formula is high enough. The non-polynomial case is also discussed and a number of test problems are finally presented in order to compare the behavior of the new methods to the theoretical results.

1. Introduction and background

We consider canonical Hamiltonian systems in the form

$$\frac{dy}{dt} = J\nabla H(y), \qquad J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix}, \qquad y(t_0) = y_0 \in \mathbb{R}^{2m}, \quad (1)$$

where $H(y)$ is a smooth real-valued function. Our interest is in researching numerical methods that provide approximations $y_n \simeq y(t_0 + nh)$ to the true solution along which the energy is precisely conserved, namely

$$H(y_n) = H(y_0), \quad \text{for all stepsizes } h \le h_0. \quad (2)$$

The study of energy-preserving methods form a branch of *geometrical numerical integration*, a research topic whose main aim is preserving qualitative features of simulated differential equations. In this context, symplectic methods have had considerable attention due to their good long-time behavior as compared to standard methods for ODEs [1–3]. A related interesting approach based upon exponential/trigonometric fitting may be found in [4–6]. Unfortunately, symplecticity cannot be fully combined with the energy preservation property [7], and this partly explains why the latter has been absent from the scene for a long time.

Among the first examples of energy-preserving methods, we mention discrete gradient schemes [8,9] which are defined by devising discrete analogs of the gradient function. The first formulae in this class had order at most two but recently discrete gradient methods of arbitrarily high order have been researched by considering the simpler case of systems with one-degree of freedom [10,11].

Here, the key tool we wish to exploit is the well-known line integral associated with conservative vector fields, such us the one defined at (1), as well as its discrete version, the so called *discrete line integral*. Interestingly, the line integral provides a manner for checking the energy conservation property, namely

$$\begin{aligned} H(y(t_1)) - H(y_0) &= \int_{y_0 \to y(t_1)} \nabla H(y)\mathrm{d}y \\ &= h\int_0^1 y'(t_0+\tau h)^T \nabla H(y(t_0+\tau h))\mathrm{d}\tau \\ &= h\int_0^1 \nabla^T H(y(t_0+\tau h)) J^T \nabla H(y(t_0+\tau h))\mathrm{d}\tau = 0, \end{aligned}$$

with $h = t_1 - t_0$, that can be easily converted into a discrete analog by considering a quadrature formula in place of the integral.

☆ Work developed within the project "Numerical methods and software for differential equations".

* Correspondence to: Dipartimento di Matematica "U. Dini", Università di Firenze, Italy.
E-mail addresses: luigi.brugnano@unifi.it (L. Brugnano), felix@dm.uniba.it (F. Iavernaro).
[1] Deceased.

0010-4655/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.cpc.2012.04.002

The discretization process requires to change the curve $y(t)$ in the phase space $\mathbb{R}^{2m}$ to a simpler curve $\sigma(t)$ (generally but not necessarily a polynomial), which is meant to yield the approximation at time $t_1 = t_0 + h$, that is $y(t_0 + h) = \sigma(t_0 + h) + O(h^{p+1})$, where p is the order of the resulting numerical method. In a certain sense, the problem of numerically solving (1) while preserving the Hamiltonian function is translated into a quadrature problem.

For example, consider the segment $\sigma(t_0+ch) = (1-c)y_0+cy_1$, with $c \in [0, 1]$, joining y_0 to an unknown point y_1 of the phase space. The line integral of $\nabla H(y)$ evaluated along σ becomes

$$H(y_1) - H(y_0) = h(y_1 - y_0)^T \int_0^1 \nabla H((1-c)y_0 + cy_1)\,\mathrm{d}c. \qquad (3)$$

Now assume that $H(y) \equiv H(q, p)$ is a polynomial of degree ν in the generalized coordinates q and in the momenta p. The integrand in (3) is a polynomial of degree $\nu - 1$ in c and can be exactly solved by any quadrature formula with abscissae $c_1 < c_2 < \cdots < c_k$ in $[0, 1]$ and weights $b_1, \ldots, b_k$, having degree of precision $d \geq \nu - 1$. We thus obtain

$$H(y_1) - H(y_0) = h(y_1 - y_0)^T \sum_{i=1}^{k} b_i \nabla H((1-c_i)y_0 + c_i y_1).$$

To get the energy conservation property we impose that $y_1 - y_0$ be orthogonal to the above sum, and in particular we choose (for the sake of generality we use $f(y)$ in place of $J\nabla H(y)$ to mean that the resulting method also makes sense when applied to a general ordinary differential equation $y' = f(y)$)

$$\begin{aligned} y_1 &= y_0 + h\sum_{i=1}^{k} b_i f(Y_i), \\ Y_i &= (1-c_i)y_0 + c_i y_1, \qquad i = 1, \ldots, k. \end{aligned} \qquad (4)$$

Formula (4) defines a Runge–Kutta method with Butcher tableau $\begin{array}{c|c} c & cb^T \\ \hline & b^T \end{array}$, where c and b are the vectors of the abscissae and weights, respectively. The stages Y_i are called *silent stages* since their presence does not affect the degree of nonlinearity of the system to be solved at each step of the integration procedure: the only unknown is y_1 and consequently (4) defines a mono-implicit method. Mono-implicit methods of Runge–Kutta type have been researched in the past by several authors (see, for example, [12–15] for their use in the solution of initial value problems).

Methods such as (4) date back to 2007 [16,17] and are called k-stage trapezoidal methods since on the one hand formula (4) reduces to the trapezoidal rule for $k = 2, c_1 = 0, c_2 = 1$ and $b_1 = b_2 = 1/2$ and on the other hand all other methods become trapezoidal in the linear case under assumption that their order is at least 2.

Generalizations of (4) to higher orders require the use of a polynomial σ of higher degree and are based upon the same reasoning as the one discussed above. Up to now, such extensions have taken the form of Runge–Kutta methods [18–20]. It has been shown that choosing a proper polynomial σ of degree s yields a Runge–Kutta method of order $2s$ with $k \geq s$ stages. The peculiarity of such energy-preserving formulae, called Hamiltonian Boundary Value Methods (HBVMs), is that the associated Butcher matrix has rank s rather than k, since $k - s$ stages may be cast as linear combinations of the remaining ones, similarly to the stages Y_i in (4).[2] As a consequence, the nonlinear system to be solved at each step has dimension $2ms$ instead of $2mk$, which is better visualized by recasting the method in block-BVM form [18] (see also [22]).

In the case where $H(y)$ is not a polynomial, one can still get a *practical* energy conservation by choosing k large enough so that the quadrature formula approximates the corresponding integral to within machine precision. Strictly speaking, taking the limit as $k \to \infty$ leads to limit formulae where the integrals come back into play in place of the sums. For example, letting $k \to \infty$ in (4) just means that the integral in (3) must not be discretized at all, which would yield the *Averaged Vector Field* method $y_1 = y_0 + h\int_0^1 f((1-c)y_0 + cy_1)\,\mathrm{d}c$, (see [23–25] for details on such limit formulae and [19] for their relation with HBVMs).

In this paper we start an investigation that follows a different route. Unlike the case with HBVMs, we want now to take advantage of the previously computed approximations to extend the class (4) in such a way to increase the order of the resulting methods, much as the class of linear multistep method may be viewed as a generalization of (linear) one-step methods. The general question we want to address is whether there exist k-step mono-implicit energy-preserving methods of order greater than two. Clearly, the main motivation is to reduce the computational cost associated with the implementation of HBVMs.

The purpose of the present paper is to give an affirmative answer to this issue in the case $k = 2$. More specifically, the method resulting from our analysis, summarized by formula (15), may be thought of as a nearly linear two-step method in that it is the sum of a fourth-order linear two-step method, formula (17), plus a nonlinear correction of higher order.[3]

The paper is organized as follows. In Section 2 we introduce the general formulation of the method, by which we mean that the integrals are initially not discretized to maintain the theory at a general level. In this section and in Appendix we report a brief description of the HBVM of order four, since its properties will be later exploited to deduce the order of the new method: this will be the subject of Section 3. Section 4 is devoted to the discretization of the integrals, which will produce the final form of the methods making them ready for implementation. A few test problems are presented in Section 5 to confirm the theoretical results.

2. Definition of the method

Suppose that y_1 is an approximation to the true solution $y(t)$ at time $t_1 = t_0 + h$, where $h > 0$ is the stepsize of integration. More precisely, we assume that

(A$_1$) $y(t_1) = y_1 + O(h^{p+1})$ with $p \geq 4$;
(A$_2$) $H(y_1) = H(y_0)$, which means that y_1 lies on the very same manifold $H(y) = H(y_0)$ as the continuous solution $y(t)$.

The two above assumptions are fulfilled if, for example, we compute y_1 by means of a HBVM (or an ∞-HBVM [19]) of order $p \geq 4$. The new approximation $y_2 \simeq y(t_2) \equiv y(t_0 + 2h)$ is constructed as follows.

Consider the quadratic polynomial $\sigma(t_0+2\tau h)$ that interpolates the set of data $\{(t_0 + jh, y_j)\}_{j=0,1,2}$. Expanded along the Newton basis $\{P_j(\tau)\}$ defined on the nodes $\tau_0 = 0, \tau_1 = \frac{1}{2}, \tau_2 = 1$, the polynomial σ takes the form (for convenience we order the nodes as τ_0, τ_2, τ_1)

$$\sigma(t_0 + 2\tau h) = y_0 + (y_2 - y_0)\tau + 2(y_2 - 2y_1 + y_0)\tau(\tau - 1). \qquad (5)$$

As τ ranges in the interval $[0, 1]$, the vector $\gamma(\tau) \equiv \sigma(t_0 + 2\tau h)$ describes a curve in the phase space $\mathbb{R}^{2m}$. The line integral of the

[2] A documentation about HBVMs, Matlab codes, and a complete set of references is available at the url [21].

[3] Here the term *linear* refers to the linear combination involving the vector field $\nabla H(y)$. Notice however that, as is the case with one-leg methods, each function is evaluated at points that are linear combinations of the two previous computed approximations and the current one.

conservative vector field $\nabla H(y)$ along the curve γ will match the variation of the energy function $H(y)$, that is

$$\begin{aligned} H(y_2) - H(y_0) &= \int_{y_0 \to y_2} \nabla H(y)\mathrm{d}y \\ &= \int_0^1 \left[\gamma'(\tau)\right]^T \nabla H(\gamma(\tau))\,\mathrm{d}\tau \\ &= (y_2 - y_0)^T \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau + 2(y_2 - 2y_1 + y_0)^T \\ &\quad \times \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau. \end{aligned}$$

The energy conservation condition $H(y_2) = H(y_0)$ yields the following equation in the unknown $z \equiv y_2$

$$(z - y_0)^T \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau = -2(z - 2y_1 + y_0)^T \times \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau. \quad (6)$$

The method we are interested in has the form $y_2 = \Psi_h(y_0, y_1)$, where Ψ_h is implicitly defined by the following nonlinear equation in the unknown z

$$\begin{aligned} z &= y_0 + 2hJa(z) + \frac{r(z)}{\|a(z)\|^2}a(z), \quad \text{with } a(z) \\ &= \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau, \end{aligned} \quad (7)$$

where, here and in the following, $\|\cdot\|$ denotes the Euclidean norm and the residual $r(z)$ is defined as

$$r(z) \equiv -2(z - 2y_1 + y_0)^T \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau. \quad (8)$$

A direct computation shows that any solution z^* of (7) also satisfies (6). In the next section we will show that (7) admits a unique solution $y_2 \equiv z^*$ satisfying the order condition $y_2 = y(t_0 + 2h) + O(h^5)$. Such a result will be derived by regarding (7) as a perturbation of the HBVM of order four and, in turn, by comparing the two associated numerical solutions. The HBVM of order four (see [17,18]), applied on the interval $[t_0, t_2]$ of length $2h$, is the one-step method

$$\begin{cases} u_2 - y_0 = 2hJ \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau, \\ u_2 - 2u_1 + y_0 = 3hJ \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau, \end{cases} \quad (9)$$

where we have used u_1 and u_2 in place of y_1 and y_2 to denote the approximations generated by the method at times t_1 and t_2 respectively. In particular, it may be shown that $u_2 = y(t_0 + 2h) + O(h^5)$ and $u_1 = y(t_0 + h) + O(h^4)$. To better explain the genesis of such a formula and how it relates to (7), a brief description of the HBVM of order four has been introduced in Appendix.

Evidently, the implementation of (7) on a computer cannot leave out of consideration the issue of solving the two integrals. To maintain the theory at a general level, we will defer this question to Section 4 (see also Appendix for the related problem concerning (9)).

3. Analysis of the method

Results on the existence and uniqueness of a solution of (7) as well as on its order of accuracy will be derived by first analyzing the simpler nonlinear system

$$z = y_0 + 2hJa(z), \quad \text{with } a(z) = \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau, \quad (10)$$

obtained by neglecting the correction term $\frac{r(z)}{\|a(z)\|^2}a(z)$. For $z \in \mathbb{R}^{2m}$ we set (see (5))

$$\gamma_z(\tau) = y_0 + (z - y_0)\tau + 2(z - 2y_1 + y_0)\tau(\tau - 1), \quad (11)$$

and (see (10))

$$\Phi(z) = y_0 + 2hJa(z). \quad (12)$$

Remark 1. The method defined at (10) also makes sense when applied to a general initial value problem $y'(t) = f(y(t))$. In such a case, since $\gamma(\tau)$ may be interpreted as a continuous linear combination of the approximations at previous grid points y_0, y_1 and the current approximation y_2, considering that $Ja(z) = \int_0^1 f(\gamma(\tau))\,\mathrm{d}\tau$, the method may be thought of as a generalization of one-leg methods.

Lemma 1. *There exist positive constants ρ and h_0 such that, for $h \le h_0$, system (10) admits a unique solution $\hat{z}$ in the ball $B(y_0, \rho)$ of center y_0 and radius ρ.*

Proof. We show that constants $h_0, \rho > 0$ exist such that the function defined in (12) satisfies the following two conditions for $h \le h_0$:

(a) $\Phi(z)$ is a contraction on $B(y_0, \rho)$, namely

$$\forall z, w \in B(y_0, \rho), \quad \|\Phi(z) - \Phi(w)\| \le L\|z - w\|, \quad \text{with } L < 1;$$

(b) $\|\Phi(y_0) - y_0\| \le (1 - L)\rho$.

The contraction mapping theorem can then be applied to obtain the assertion.

Let $B(y_0, \rho)$ be a ball centered at y_0 with radius ρ. We can choose h_0' and ρ small enough that the image set $\Omega = \{\gamma_z(\tau) : \tau \in [0, 1],\ z \in B(y_0, \rho),\ h \le h_0'\}$ is entirely contained in a ball $B(y_0, \rho')$ which, in turn, is contained in the domain of $\nabla^2 H(y)$.[4] We set

$$M_\rho = \max_{w \in B(y_0, \rho')} \left\|\nabla^2 H(w)\right\|.$$

From (10) and (11) we have

$$\frac{\partial a(z)}{\partial z} = \int_0^1 \nabla^2 H(\gamma_z(\tau))\frac{\partial \gamma_z}{\partial z}\,\mathrm{d}\tau = \int_0^1 \nabla^2 H(\gamma_z(\tau))\,\tau(2\tau - 1)\,\mathrm{d}\tau$$

and hence

$$\left\|\frac{\partial a(z)}{\partial z}\right\| \le M_\rho \int_0^1 \tau|2\tau - 1|\,\mathrm{d}\tau = \frac{1}{4}M_\rho.$$

Consequently (a) is satisfied by choosing

$$L = \frac{h}{2}M_\rho \quad (13)$$

and $h_0 < \min\{\frac{2}{M_\rho}, h_0'\}$. Concerning (b), we observe that

$$\begin{aligned} \Phi(y_0) - y_0 &= 2hJa(y_0) \\ &= 2hJ \int_0^1 \nabla H(y_0 + 4(y_0 - y_1)\tau(\tau - 1))\,\mathrm{d}\tau, \end{aligned}$$

hence $\|\Phi(y_0) - y_0\| = 2h\|a(y_0)\|$ with $\|a(y_0)\|$ bounded with respect to h. Since L vanishes with h (see (13)), we can always tune h_0 in such a way that $2h\|a(y_0)\| \le (1 - L)\rho$. □

[4] Notice that, by definition, the set Ω is an open simply connected subset of $\mathbb{R}^{2m}$ containing $B(y_0, \rho)$ while, from the assumption (A_1), decreasing h causes the point y_1 to approach y_0.

Lemma 2. *The solution $\hat z$ of (10) satisfies $y(t+2h)-\hat z = O(h^5)$.*

Proof. Under the assumption (A_1), (10) may be regarded as a perturbation of system (9), since y_1 and u_1 are $O(h^5)$ and $O(h^4)$ close to $y(t+h)$ respectively.[5] Since $u_2 = y(t+2h)+O(h^5)$, we can estimate the accuracy of $\hat z$ as an approximation of $y(t+2h)$ by evaluating its distance from u_2.

Let $\tilde\gamma(\tau)$ be the underlying quadratic curve associated with the HBVM defined by (9), namely

$$\tilde\gamma(\tau) \equiv y_0 + (u_2 - y_0)\tau + 2(u_2 - 2u_1 + y_0)\tau(\tau-1). \tag{14}$$

Considering that (see (11))

$$\begin{aligned}\gamma_{u_2}(\tau) &\equiv y_0 + (u_2 - y_0)\tau + 2(u_2 - 2y_1 + y_0)\tau(\tau-1)\\ &= \tilde\gamma(\tau) + 4(u_1 - y_1)\tau(\tau-1),\end{aligned}$$

from the first equation in (9) and (12) we get

$$\begin{aligned}\Phi(u_2) &= y_0 + 2hJ\int_0^1 \nabla H(\gamma_{u_2}(\tau))\,d\tau\\ &= y_0 + 2hJ\int_0^1 \nabla H(\tilde\gamma(\tau))\,d\tau + 8hJ\\ &\quad\times\int_0^1 \nabla^2 H(\tilde\gamma(\tau))\tau(\tau-1)\,d\tau\cdot(u_1-y_1)\\ &\quad + O(\|u_1-y_1\|^2)\\ &= u_2 + O(h^5).\end{aligned}$$

If h is small enough, u_2 will be inside the ball $B(y_0,\rho)$ defined in Lemma 1. The Lipschitz condition yields (see (13))

$$\|\hat z - u_2\| = \|\Phi(\hat z) - \Phi(u_2) + O(h^5)\| \le \frac{h}{2}M_\rho\|\hat z - u_2\| + O(h^5),$$

and hence $\|\hat z - u_2\| = O(h^5)$. □

The above result states that (10) defines a method of order 4 which is a simplified version of our conservative method defined at (7). In Section 5 the behavior of these two methods will be compared on a set of test problems. We stress that (10) is not conservative and, in fact, it is the introduction of a suitable correction term that restores the conservation property without causing a loss of order, as the next theorem shows.

Theorem 1. *Under the assumption (A_1), for h small enough, equation (7) admits a unique solution z^* satisfying $y(t+2h)-z^* = O(h^5)$.*

Proof. Consider the solution $\hat z$ of system (10). We have (see (14))

$$\begin{aligned}\gamma_{\hat z}(\tau) - \tilde\gamma(\tau) &= (\hat z - u_2)\tau(2\tau-1) + 4(u_1-y_1)\tau(\tau-1)\\ &= O(h^5),\end{aligned}$$

and

$$\hat z - 2y_1 + y_0 = u_2 - 2u_1 + y_0 + O(h^5).$$

Hence, by virtue of (9),

$$\begin{aligned}r(\hat z) &= -2\left[(u_2 - 2u_1 + y_0) + O(h^5)\right]^T\\ &\quad\times\left[\int_0^1 (2\tau-1)\nabla H(\tilde\gamma(\tau))\,d\tau + O(h^5)\right] = O(h^5).\end{aligned}$$

Since $a(\hat z)$ is bounded with respect to h, it follows that, in a neighborhood of $\hat z$, system (7) may be regarded as a perturbation of system (10), the perturbation term being $R(z,h) \equiv \frac{r(z)}{\|a(z)\|^2}a(z)$.

[5] This also implies that $u_1 - y_1 = O(h^4)$.

Consider the ball $B(\hat z, R(\hat z,h))$: since $\hat z = y_0 + O(h)$, and $R(\hat z,h) = O(h^5)$, this ball is contained in $B(y_0,\rho)$ defined in Lemma 1 and the perturbed function $\Phi(z)+R(z,h)$ is a contraction therein, provided h is small enough. Evaluating the right-hand side of (7) at $z=\hat z$ we get

$$y_0 + 2hJa(\hat z) + R(\hat z,h) = \hat z + R(\hat z,h),$$

which means that property (b) listed in the proof of Lemma 1, with $\hat z$ in place of y_0, holds true for the perturbed function $y_0 + 2hJa(z) + R(z,h)$, and the contraction mapping theorem may be again exploited to deduce the assertion. □

4. Discretization

As was stressed in Section 2, formula (7) is not operative unless a technique to solve the two integrals is taken into account. The most obvious choice is to compute the integrals by means of a suitable quadrature formula which may be assumed exact in the case where the Hamiltonian function is a polynomial, and to provide an approximation to within machine precision in all other cases.

Hereafter we assume that $H(q,p)$ is a polynomial in q and p of degree ν. Since $\gamma(\tau)$ has degree two, it follows that the integrand functions appearing in the definitions of $a(z)$ and $r(z)$ at (7) and (8) have degree $2\nu-2$ and $2\nu-1$ respectively and can be solved by any quadrature formula with abscissae $c_1 < c_2 < \cdots < c_k$ in $[0,1]$ and weights $b_1,\dots,b_k$, having degree of precision $d \ge 2\nu-1$. In place of (7) we now consider the equivalent form suitable for implementation

$$y_2 = y_0 + 2hJ\sum_{i=1}^k b_i\nabla H(\gamma(c_i)) + G(y_0,y_1,y_2), \tag{15}$$

where

$$\begin{aligned}G(y_0,y_1,y_2) &= \frac{-2(y_2-2y_1+y_0)^T\sum_{i=1}^k b_i(2c_i-1)\nabla H(\gamma(c_i))}{\left\|\sum_{i=1}^k b_i\nabla H(\gamma(c_i))\right\|_2^2}\\ &\quad\times\sum_{i=1}^k b_i\nabla H(\gamma(c_i)).\end{aligned}$$

Notice that from (5) we get

$$\gamma(c_i) = (1-3c_i+2c_i^2)y_0 + 4c_i(1-c_i)y_1 + c_i(2c_i-1)y_2, \tag{16}$$

that is, $\gamma(c_i)$ is a linear combination, actually a weighted average, of the approximations y_0, y_1 and y_2. Therefore, since $G(y_0,y_1,y_2) = O(h^5)$ (see Lemma 2 and Theorem 1), we may look at this term as a nonlinear correction of the generalized linear multistep method

$$y_2 = y_0 + 2hJ\sum_{i=1}^k b_i\nabla H(\gamma(c_i)). \tag{17}$$

Example 1. If $H(q,p)$ is quadratic, we can choose $k=3$, $c_1=0$, $c_2=\frac12$, $c_3=1$, $b_1=b_3=\frac16$ and $b_2=\frac23$, that is we can use Simpson's quadrature formula to compute the integrals in (7) and (8). Since, in such a case, $\gamma(c_i)=y_{i-1}$, method (17) becomes

$$y_2 = y_0 + \frac{h}{3}J\left(\nabla H(y_0) + 4\nabla H(y_1) + \nabla H(y_2)\right),$$

that is, the standard Milne–Simpson's method.

In all other cases $\gamma(c_i)$ will differ in general from y_j, $j=1,2,3$ and may be regarded as an off-point entry in formula (17). In the sequel we will denote the method defined at (15) by M_k and its linear part, defined at (17), by M_k'. Of course, the choice of the abscissae distribution influences the energy preserving properties of the method M_k, as is indicated in Table 1.

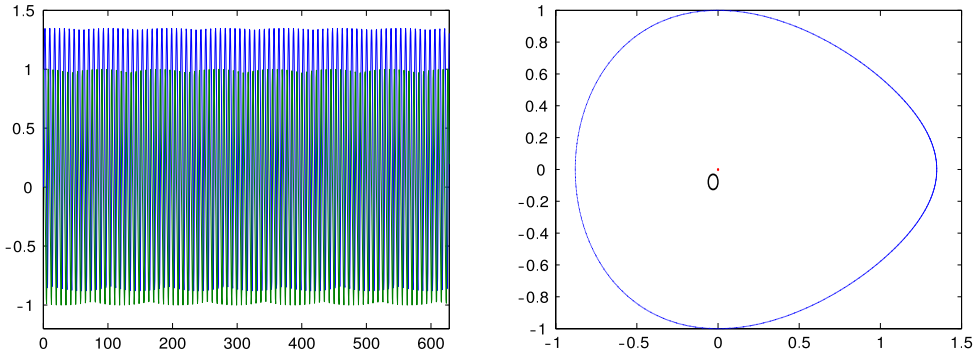

Fig. 1. Numerical solution (q_n, p_n) versus time t_n (left picture) and on the phase plane (right picture). Parameters: initial condition $y_0 = [0,\ 1]$; stepsize $h = 0.5$; integration interval $[0, 200\pi]$.

Table 1
Energy preserving properties of method M_k for some well-known distributions of the nodes $\{c_i\}$.

Abscissae distribution:	Uniform	Lobatto	Gauss
Energy preserving when:	$\deg H \le \lceil \frac{k}{2} \rceil$	$\deg H \le k-1$	$\deg H \le k$

5. Numerical tests

Hereafter we implement the order four method M_k on a few Hamiltonian problems to show that the numerical results are consistent with the theory presented in Section 3. In particular, in the first two problems the Hamiltonian function is a polynomial of degree three and six respectively, while the last numerical test reports the behavior of the new method on a non-polynomial problem also in comparison with the associated HBVM of order four (9).

Each step of the integration procedure requires the solution of a nonlinear system, in the unknown y_2, represented by (15) for the method M_k and (17) for the method M'_k. The easiest way (although not the most efficient one) to find out a solution is by means of fixed-point iteration that, in the case of the method M_k, reads

$$z_{s+1} = y_0 + 2hJ \sum_{i=1}^{k} b_i \nabla H(\gamma_{z_s}(c_i)) + G(y_0, y_1, z_s),$$
$$s = 1, 2, \ldots, \tag{18}$$

where γ_z is defined at (11) and z_0 is an initial approximation of y_2 which is then refined by setting $y_2 = z_{\bar{s}}$ with $z_{\bar{s}} \simeq \lim_{s\to\infty} z_s$. From Theorem 1 and the preceding lemmas we deduce that such a limit always exists provided that h is small enough. The value of z_0 could be retrieved via an extrapolation based on the previous computed points and/or by allowing a small fixed number of preliminary iterations in the form (18) but with the terms $\nabla H(\gamma_{z_s}(c_i))$ replaced by approximations obtained by quadratic interpolation based on the values $\nabla H(y_0)$, $\nabla H(y_1)$ and $\nabla H(z_s)$. Since the first two values remain the same during the iteration, performing this prediction only costs one function evaluation per step and results in a considerable reduction of the total number of function evaluations needed to advance the solution.

We will consider a Lobatto distribution with an odd number k of abscissae $\{c_i\}$. In fact, if k is odd, since $y_0 = \gamma(0) = \gamma(c_1)$ and $y_1 = \gamma(\frac{1}{2}) = \gamma(c_{\lceil \frac{k}{2} \rceil})$, we save two function evaluations during the iteration (18). Finally, as was emphasized at the beginning of Section 2, we use a one-step method to produce the very first approximation $y_1 \simeq y(t_0 + h)$ and in particular, to obtain both the order and the energy conservation property at time $t_1 = t_0 + h$, we have chosen the HBVM formula of order four (9) with the integrals discretized by a Lobatto quadrature (see Appendix).

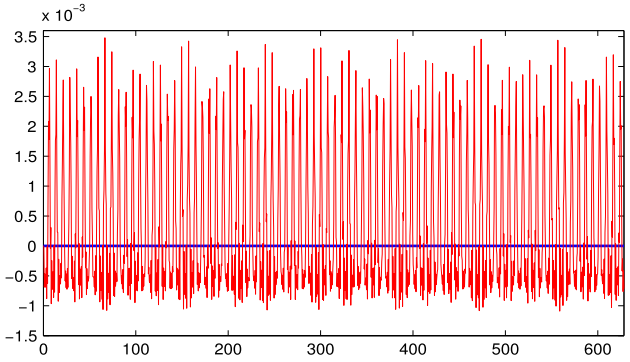

Fig. 2. Hamiltonian function evaluated along the numerical solution (p_n, q_n) (horizontal line) and along the numerical solution (p'_n, q'_n) (irregularly oscillating line).

5.1. Test problem 1

The Hamiltonian function

$$H(q, p) = \frac{1}{2}p^2 + \frac{1}{2}q^2 - \frac{1}{6}q^3 \tag{19}$$

defines the cubic pendulum equation. We can solve it by using five Lobatto nodes to discretize the integrals in (7), thus getting the method M_5. The corresponding numerical solution, denoted by (q_n, p_n), is plotted in Fig. 1. For comparison purposes we also compute the numerical solution (q'_n, p'_n) provided by the fourth-order method, say M'_5, obtained by neglecting in (7) the correction term, that is by posing $r(z) \equiv 0$. Fig. 2 clearly shows the energy conservation property, while Table 2 summarizes the convergence properties of the two methods.

5.2. Test problem 2

The Hamiltonian function

$$H(p, q) = \frac{1}{3}p^3 - \frac{1}{2}p + \frac{1}{30}q^6 + \frac{1}{4}q^4 - \frac{1}{3}q^3 + \frac{1}{6} \tag{20}$$

has been proposed in [26] to show that symmetric methods may suffer from the energy drift phenomenon even when applied to reversible systems, that is when $H(-p, q) = H(p, q)$.[6] For our experiment, we will use $y_0 = [0.2,\ 0.5]$ as initial condition.

Since $\deg(H(q, p)) = 6$, we need a Lobatto quadrature based on at least seven nodes to assure that the integrals in (7) are computed

[6] In fact, the authors show that the system deriving from (20) is equivalent to a reversible system (see also [27,28] for a discussion on the integration of reversible Hamiltonian systems by symmetric methods).

Table 2
Methods M_5 (with correction term) and M_5' (without correction term) are implemented on the cubic pendulum equation (19) on the time interval $[0,\ 10]$ for several values of the stepsize h. The order of convergence is numerically evaluated by means of the formula $\log_2 \frac{\text{error}(\frac{h}{2})}{\text{error}(h)}$. As was expected, the maximum displacement of the numerical Hamiltonian $H(y_n)$ from the theoretical value $H(y_0)$ is close to the machine precision for the method M_5, independently of the stepsize h used.

h	Method M_5			Method M_5'		
	Error	Order	$\max \lvert H(y_n) - H(y_0)\rvert$	Error	Order	$\max \lvert H(y_n') - H(y_0)\rvert$
1	$3.1 \cdot 10^{-2}$		$2.5 \cdot 10^{-15}$	$1.1 \cdot 10^{-1}$		$1.1008 \cdot 10^{-1}$
2^{-1}	$3.8 \cdot 10^{-4}$	6.373	$1.9 \cdot 10^{-15}$	$3.1 \cdot 10^{-3}$	5.183	$2.9680 \cdot 10^{-3}$
2^{-2}	$2.6 \cdot 10^{-5}$	3.866	$1.5 \cdot 10^{-15}$	$2.5 \cdot 10^{-4}$	3.655	$1.5755 \cdot 10^{-4}$
2^{-3}	$1.6 \cdot 10^{-6}$	4.059	$8.8 \cdot 10^{-16}$	$1.8 \cdot 10^{-5}$	3.811	$8.5163 \cdot 10^{-6}$
2^{-4}	$9.5 \cdot 10^{-8}$	4.032	$9.9 \cdot 10^{-16}$	$1.2 \cdot 10^{-6}$	3.905	$4.8883 \cdot 10^{-7}$
2^{-5}	$5.9 \cdot 10^{-9}$	4.017	$1.1 \cdot 10^{-15}$	$7.6 \cdot 10^{-8}$	3.952	$2.9131 \cdot 10^{-8}$
2^{-6}	$3.6 \cdot 10^{-10}$	4.008	$1.1 \cdot 10^{-15}$	$4.9 \cdot 10^{-9}$	3.976	$1.7771 \cdot 10^{-9}$
2^{-7}	$2.3 \cdot 10^{-11}$	4.004	$2.3 \cdot 10^{-15}$	$3.1 \cdot 10^{-10}$	3.988	$1.0968 \cdot 10^{-10}$
2^{-8}	$1.4 \cdot 10^{-12}$	4.006	$2.4 \cdot 10^{-15}$	$1.9 \cdot 10^{-11}$	3.994	$6.8121 \cdot 10^{-12}$

exactly. Therefore we solve (20) by method M_7. For comparison purposes, it is also interesting to show the dynamics of the symmetric non-conservative method M_7'. Fig. 3 displays the results obtained by the two methods implemented with stepsize $h = \frac{1}{10}$ over the interval $[0,\ 10^3]$. In particular, the numerical trajectories generated by method M_7' and M_7, are reported in the left-top and left-bottom pictures respectively, while the right picture reports the corresponding error in the Hamiltonian function evaluated along the two numerical solutions, namely $|H(y_n) - H(y_0)|$.

Evidently, the numerical solution produced by M_7' rapidly departs from the level curve $H(q, p) = H(q_0, p_0)$ but it remain eventually bounded and the points (q_n, p_n) seem to densely fill a bounded region of the phase plane.

On the contrary, since the degree of freedom of the present problem is one, the points (q_n, p_n) produced by M_7 lie on the very same continuous trajectory covered by $y(t)$: this is also confirmed by looking at the bottom graph in the right picture.

Table 3 shows the behavior of method M_7 applied to problem (20) as the stepsizes h goes to zero. Notice the $O(h^5)$ rate of convergence to zero for the residual function $r(z)$ in (8).

5.3. Test problem 3

We finally consider the non-polynomial Hamiltonian function

$$H(q_1, q_2, p_1, p_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} \tag{21}$$

that defines the well known Kepler problem, namely the motion of two masses under the action of their mutual gravitational attraction. Taking as initial condition

$$(q_1(0), q_2(0), p_1(0), p_2(0)) = \left(1 - e,\quad 0,\quad 0,\quad \sqrt{\frac{1+e}{1-e}}\right)^T \tag{22}$$

yields an elliptic periodic orbit of period 2π and eccentricity $e \in [0, 1)$. We have chosen $e = 0.6$. Though the vector field fails to be a polynomial in q_1 and q_2, we can plan to use a sufficiently large number of quadrature nodes to discretize the integrals in (7) so that the corresponding accuracy is within the machine precision. Under this assumption, and taking aside the effect of the floating point arithmetic, the computer will make no difference between the conservative formulae (7) and their discrete counterparts.

The left picture in Fig. 4 explains the above argument. It reports the error $|H(y_n) - H(y_0)|$ in the Hamiltonian function for various choices of the number of Lobatto nodes, and precisely $k = 3, 5, 7, 9$. We see that the error decreases quickly as the number of nodes is incremented and for $k = 9$ it is within the epsilon machine.[7]

The use of finite arithmetic may sometimes cause a mild numerical drift of the energy over long times, like the one shown in the upper line in the right picture of Fig. 4. This is due to the fact that on a computer the numerical solution satisfy the conservation relation $H(y_n) = H(y_0)$ up to machine precision times the conditioning number of the nonlinear system that is to be solved at each step.

To prevent the accumulation of roundoff errors we may apply a simple and costless *correction* technique on the approximation y_n which consists in a single step of a gradient descent method (see also [29]). More precisely, the corrected solution y_n^* is defined by

$$y_n^* = y_n - \alpha \frac{\nabla H(y_n)}{\|\nabla H(y_n)\|}, \quad \text{with } \alpha = \frac{H(y_n) - H(y_0)}{\|\nabla H(y_n)\|}, \tag{23}$$

which stems from choosing as α the value that minimizes the linear part of the function $F(\alpha) = H(y_n - \alpha \frac{\nabla H(y_n)}{\|\nabla H(y_n)\|}) - H(y_0)$. The bottom line in the right picture of Fig. 4 shows the energy conservation property of the corrected solution.

5.4. A comparison

The analysis of a more powerful technique to solve the nonlinear systems associated with the new methods, their extension to a number of steps greater than two as well as the stepsize variation strategy, will be the subject of a future investigation.[8] Nevertheless, it is interesting, even at this early stage, to compare the behavior of the new method M_k to the related HBVM of order four (9), on the basis of their implementation carried out by a fixed-point iteration procedure coupled with a constant stepsize. To this end, we have applied the two order four (practically) energy-preserving methods M_{11} and *HBVM* with 11 Lobatto nodes (see Appendix) to the Kepler problem (21). We integrate the Hamiltonian system over ten periods by using successively decreasing stepsizes and compute the error at the final time and the total number of function evaluation required. Fig. 5 shows that the method M_{11} allows a concrete reduction of the total number of function evaluations needed to achieve a prescribed precision in the numerical solution, which provides a preliminary hint about the potential efficiency of the new formulae. For comparison purposes we have also added the results for the Gauss method of order four (which is symplectic but not

[7] All tests were performed in Matlab using double precision arithmetic.

[8] As is the case with linear multistep methods, the use of a Newton-like procedure is highly recommended to take advantage of the fact that, in contrast to Runge–Kutta methods, the nonlinear system associated with the new methods shares the very same dimension of the underlying continuous problem.

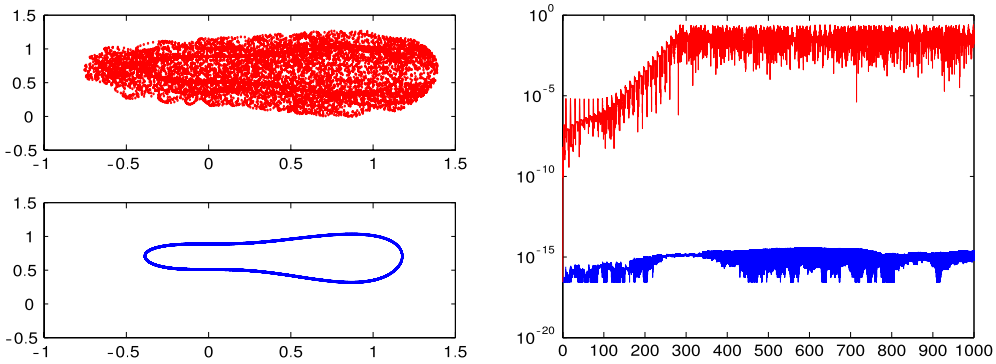

Fig. 3. Left pictures: numerical solutions in the phase plane computed by method M_7' (top picture) and M_7 (bottom picture). Right picture: error in the numerical Hamiltonian function $|H(y_n) - H(y_0)|$ produced by the two methods. Parameters: initial condition $y_0 = [0.2,\ 0.5]$; stepsize $h = 0.1$; integration interval $[0,\ 1000]$.

Table 3
Performance of method M_7 applied to problem (20), with initial condition $y_0 = [0.2,\ 0.5]$, on the time interval $[0,\ 250]$ for several values of the stepsize h, as specified in the first column. The second and third columns report the relative error in the last computed point $y_N, N = T/h$ and the corresponding order of convergence. Since the integrals appearing in (7) are precisely computed by the Lobatto quadrature formula with seven nodes, the error in the numerical Hamiltonian $H(y_N)$ is zero up to machine precision. The last two columns list the residual $r(y_N)$ defined in (8) and its order of convergence to zero.

h	Method M_7				
	Error	Order	$\lvert H(y_N) - H(y_0)\rvert$	Residual $r(y_N)$	Order of $r(y_N)$
2^{-1}	$4.47 \cdot 10^{-2}$		$1.6 \cdot 10^{-16}$	$-1.21 \cdot 10^{-03}$	
2^{-2}	$7.38 \cdot 10^{-4}$	5.920	$4.4 \cdot 10^{-16}$	$-3.23 \cdot 10^{-06}$	8.559
2^{-3}	$3.90 \cdot 10^{-5}$	4.243	$5.8 \cdot 10^{-16}$	$-2.15 \cdot 10^{-08}$	7.225
2^{-4}	$2.39 \cdot 10^{-6}$	4.027	$2.4 \cdot 10^{-16}$	$-6.61 \cdot 10^{-10}$	5.029
2^{-5}	$1.49 \cdot 10^{-7}$	4.007	$2.5 \cdot 10^{-15}$	$-2.03 \cdot 10^{-11}$	5.021
2^{-6}	$9.27 \cdot 10^{-9}$	4.002	$3.2 \cdot 10^{-15}$	$-6.27 \cdot 10^{-13}$	5.018
2^{-7}	$5.77 \cdot 10^{-10}$	4.006	$5.5 \cdot 10^{-16}$	$-2.00 \cdot 10^{-14}$	4.972
2^{-8}	$3.16 \cdot 10^{-11}$	4.188	$5.4 \cdot 10^{-15}$	$-5.36 \cdot 10^{-16}$	5.219

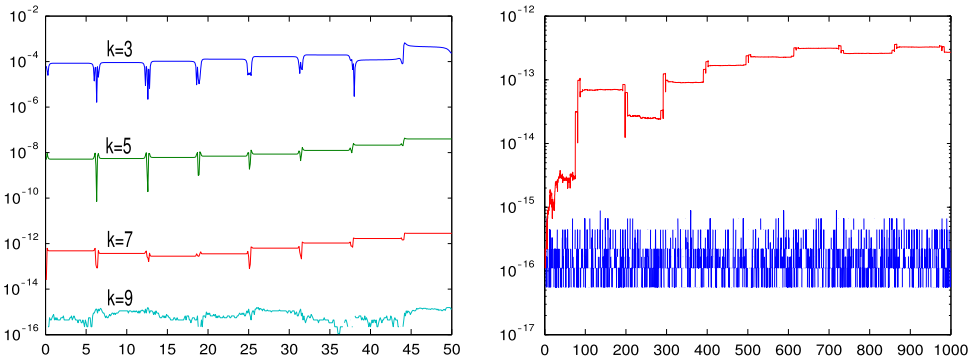

Fig. 4. Left picture. Error in the numerical Hamiltonian function $|H(y_n) - H(y_0)|$ produced by methods M_k, with $k = 3,\ 5,\ 7,\ 9$. Parameters: stepsize $h = 0.05$, integration interval $[0,\ 50]$. Right picture. Roundoff errors may cause a drift of the numerical Hamiltonian function (upper line) which can be easily taken under control by coupling the method with a costless correction procedure like the one described at (23).

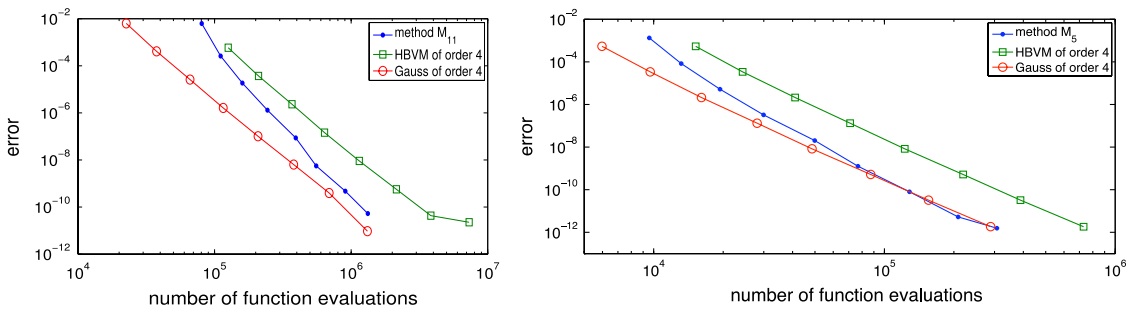

Fig. 5. Error versus number of function evaluations related to methods M_{11} (dots), the HBVM of order four with 11 Lobatto nodes (squares) and the Gauss method of order four (circles). Left picture: results for the Kepler problem (21). Right picture: results for the cubic pendulum equation (19). Both problems have been integrated on the interval $[0,\ 20\pi]$. A reference solution for the cubic pendulum problem has been computed by the Gauss method of order six with a very small stepsize.

energy preserving). That the broken line related to the Gauss method lies below the lines of the other two methods is an expected result for this non-polynomial problem: the energy conservation requirement needs that a sufficient number of nodes should be taken into account when discretizing the integrals appearing in (7)–(8) and (9) respectively.[9] In fact, a similar test conducted on the cubic pendulum equation (19), by using five Lobatto nodes, reveals a considerable reduction of the discrepancy between the three lines and, in particular, between the ones related to the method M_5 and the Gauss method (see the right picture of Fig. 5).

6. Conclusions

We have derived a family of mono-implicit methods of order four with energy-preserving properties. Each element in the family originates from a limit formula and is defined by discretizing the integral therein by means of a suitable quadrature scheme. This process assures an exact energy conservation in the case where the Hamiltonian function is a polynomial, or a conservation to within machine precision in all other cases, as is also illustrated in the numerical tests. Interestingly, each method may be conceived as a $O(h^5)$ perturbation of a two-step linear method.

Acknowledgments

We wish to acknowledge the referees for constructive comments on the first draft of the manuscript.

Appendix. HBVM of order four

This is a one-step method that may be easily retrieved from the energy conservation condition (6) which we rewrite once again by assuming u_1 and u_2 in place of y_1 and y_2 for consistency with the notation we have adopted in the paper:

$$(u_2 - y_0)^T \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau = -2(u_2 - 2u_1 + y_0)^T \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau. \tag{A.1}$$

In this case, both u_1 and u_2 are regarded as unknowns and the curve γ in the phase space is more properly defined as $\gamma(\tau) = \sigma(t_0+\tau h)$, with $\tau \in [0, 1]$, in order to cover a time interval of length h instead of $2h$ and, as usual, $u_2 = \gamma(1)$ will bring the approximation to the true solution $y(t_0 + h)$.

For (A.1) to be satisfied, we can now impose the two orthogonality conditions

$$\begin{cases} u_2 - y_0 = \eta_1 hJ \int_0^1 \nabla H(\gamma(\tau))\,\mathrm{d}\tau, \\ u_2 - 2u_1 + y_0 = \eta_2 hJ \int_0^1 (2\tau - 1)\nabla H(\gamma(\tau))\,\mathrm{d}\tau, \end{cases} \tag{A.2}$$

giving rise to a system of two block-equations. Setting the free constants η_1 and η_2 equal to 1 and 3/2, respectively, confers the highest possible order, namely 4, on the resulting method: $u_2 = y(t_0 + h) + O(h^5)$ (see [17,19] for details). Notice that the two constants appearing in (9) are scaled by a factor two with respect to the values reported above to take into account that, for convenience, we assumed a time interval of length $2h$.

Evidently, the implementation of (9) on a computer cannot leave out of consideration the issue of solving the integrals appearing in both equations. Two different situations may emerge:

(a) the Hamiltonian function $H(y)$ is a polynomial of degree ν. In such a case, the two integrals in (9) are exactly computed by a quadrature formula having degree of precision $d \geq 2\nu - 1$.
(b) $H(y)$ is not a polynomial, nor do the two integrands admit a primitive function in closed form. Again, an appropriate quadrature formula can be used to approximate the two integrals to within machine precision, so that no substantial difference is expected during the implementation process by replacing the integrals by their discrete counterparts.

Case (a) gives rise to an infinite family of Runge–Kutta methods, each depending on the specific choice (number and distribution) of nodes the quadrature formula is based upon (see [19] for a general introduction on HBVMs and [20] for their relation with standard collocation methods). For example, choosing k nodes according to a Gauss distribution over the interval $[0, 1]$ results in a method that precisely conserves the energy if applied to polynomial canonical Hamiltonian systems with $\nu \leq k$ and that becomes the classical 2-stage Gauss collocation method when $k = 2$. On the other hand, choosing a Lobatto distribution yields a Runge–Kutta method that preserves polynomial Hamiltonian functions of degree $\nu \leq k - 1$ and that becomes the Lobatto IIIA method of order four when $k = 2$.

The methods resulting from case (b) are undistinguishable from the original formulae (9) in that they are energy-preserving up to machine precision when applied to any regular canonical Hamiltonian system. Stated differently, (9) may be viewed as the limit of the family of HBVMs of order four, as the number of nodes tends to infinity. For this reason the limit formulae (9) have been called ∞-HBVM of order 4 (see [19]).

Remark 2. In the context of the present paper, y_1 being a known quantity, the unknown z in (6) cannot in general satisfy, at the same time, both orthogonality conditions in (9). However, since y_1 may be thought of as an approximation of order four to the quantity u_1 in (9), should we only impose the first orthogonality condition, namely

$$z - y_0 = 2hJa(z), \tag{A.3}$$

we would expect the residual $r(z)$ (the right hand side of (6)) to be very small.[10] This suggests that a solution to (6) that yields an approximation of high order to $y(t_0 + 2h)$ may be obtained by allowing a small deviation from orthogonality in (A.3). This is accomplished by setting $z - y_0 = 2hJa(z) + \delta a(z)$, and by tuning the perturbation parameter δ in such a way that (6) be satisfied: this evidently gives $\delta = \frac{r(z)}{\|a(z)\|^2}$ and we arrive at (7).

References

[1] R.D. Ruth, IEEE Trans. Nucl. Sci. 30 (4) (1983) 2669–2671.
[2] K. Feng, Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations, Science Press, Beijing, 1985, pp. 42–58.
[3] B. Leimkuhler, S. Reich, Simulating Hamiltonian Dynamics, Cambridge University Press, Cambridge, 2004, p. 379.
[4] L.Gr. Ixaru, G. Vanden Berghe, Exponential Fitting, in: Mathematics and its Applications, vol. 568, Kluwer Academic Publishers, Dordrecht, 2004, p. 308.
[5] G. Vanden Berghe, M. Van Daele, J. Numer. Anal. Ind. Appl. Math. 1 (2006) 237–251.
[6] T.E. Simos, Comput. Phys. Comm. 178 (2008) 199–207.
[7] Z. Ge, J.E. Marsden, Phys. Lett. A 133 (1988) 134–139.
[8] O. Gonzales, J. Nonlinear Sci. 6 (1996) 449–467.
[9] R.I. McLachlan, G.R.W. Quispel, N. Robidoux, R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci. 357 (1999) 1021–1045.
[10] J.L. Cieśliński, B. Ratkiewicz, Phys. Rev. E 81 (2010) 016704.

[9] Actually, the choice of eleven nodes is quite conservative. When the stepsize is small, a practical conservation of energy is attained with a fewer number of nodes. This expedient has not been considered in the numerical test.

[10] By exploiting the result in Lemma 2, it is not difficult to show that actually (A.3) implies $r(z) = O(h^5)$. This aspect is further emphasized in the numerical test section (see Table 3).

[11] J.L. Cieśliński, B. Ratkiewicz, Comput. Phys. Comm. 183 (3) (2012) 617–627.
[12] J.R. Cash, J. ACM 22 (4) (1975) 504–511.
[13] W.M.G. van Bokhoven, BIT 20 (1) (1980) 34–43.
[14] J.R. Cash, A. Singhal, IMA J. Numer. Anal. 2 (2) (1982) 211–227.
[15] K. Burrage, F.H. Chipman, P.H. Muir, SIAM J. Numer. Anal. 31 (3) (1994) 876–891.
[16] F. Iavernaro, B. Pace, AIP Conf. Proc. 936 (2007) 603–606.
[17] F. Iavernaro, D. Trigiante, J. Numer. Anal. Ind. Appl. Math. 4 (1–2) (2009) 87–101.
[18] L. Brugnano, F. Iavernaro, D. Trigiante, Analysis of Hamiltonian boundary value methods (HBVMs): a class of energy-preserving Runge–Kutta methods for the numerical solution of polynomial Hamiltonian dynamical systems, 2009 (submitted for publication). arXiv:0909.5659.
[19] L. Brugnano, F. Iavernaro, D. Trigiante, J. Numer. Anal. Ind. Appl. Math. 5 (1–2) (2010) 17–37.
[20] L. Brugnano, F. Iavernaro, D. Trigiante, Appl. Math. Comput. 218 (2012) 8053–8063.
[21] L. Brugnano, F. Iavernaro, D. Trigiante, The Hamiltonian BVMs (HBVMs) homepage. arXiv:1002.2757, URL: http://www.math.unifi.it/~brugnano/HBVM/.
[22] L. Brugnano, F. Iavernaro, D. Trigiante, J. Comput. Appl. Math. 236 (2011) 375–383.
[23] E. Celledoni, R.I. McLachlan, D. McLaren, B. Owren, G.R.W. Quispel, W.M. Wright, ESAIM: M2AN Math. Model. Numer. Anal. 43 (2009) 645–649.
[24] G.R.W. Quispel, D.I. McLaren, J. Phys. A 41 (4) (2008) 045206.
[25] E. Hairer, J. Numer. Anal. Ind. Appl. Math. 5 (1–2) (2010) 73–84.
[26] E. Faou, E. Hairer, T.-L. Pham, BIT 44 (2004) 699–709.
[27] L. Brugnano, D. Trigiante, J. Numer. Anal. Ind. Appl. Math. 4 (3–4) (2009) 153–170.
[28] R.I. McLachlan, M. Perlmutter, J. Phys. A 37 (45) (2004) 593–598.
[29] L. Brugnano, F. Iavernaro, T. Susca, AIP Conf. Proc. 1168 (2009) 723–726.