European Society of Computational Methods in Sciences and Engineering (ESCMSE)

Journal of Numerical Analysis, Industrial and Applied Mathematics (JNAIAM)
vol. 5, no. 1-2, 2010, pp. 17-37
ISSN 1790–8140

Hamiltonian Boundary Value Methods (Energy Preserving Discrete Line Integral Methods) [1] [2]

Luigi Brugnano[3]

Dipartimento di Matematica "U. Dini", Università di Firenze
Viale Morgagni 67/A, I-50134 Firenze, Italy

Felice Iavernaro[4]

Dipartimento di Matematica, Università di Bari
Via Orabona 4, I-70125 Bari, Italy

Donato Trigiante[5]

Dipartimento di Energetica "S.Stecco", Università di Firenze
Via Lombroso 6/17, I-50134 Firenze, Italy

Received October 25, 2009; accepted in revised form April 15, 2010.

Abstract: Recently, a new family of integrators (Hamiltonian Boundary Value Methods) has been introduced, which is able to precisely conserve the energy function of polynomial Hamiltonian systems and to provide a *practical* conservation of the energy in the non-polynomial case.
We settle the definition and the theory of such methods in a more general framework. Our aim is on the one hand to give account of their good behavior when applied to general Hamiltonian systems and, on the other hand, to find out what are the *optimal* formulae, in relation to the choice of the polynomial basis and of the distribution of the nodes. Such analysis is based upon the notion of *extended collocation conditions* and the definition of *discrete line integral*, and is carried out by looking at the limit of such family of methods as the number of the so called *silent stages* tends to infinity.

Keywords: Hamiltonian problems, exact conservation of the Hamiltonian, energy conservation, Hamiltonian Boundary Value Methods, HBVMs, discrete line integral.

Mathematics Subject Classification: 65P10, 65L05.

1 Introduction

We consider canonical Hamiltonian problems in the form

$$\dot{y} = J\nabla H(y), \qquad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

[1] Published electronically October 15, 2010
[2] Work developed within the project "Numerical methods and software for differential equations".
[3] E-mail: luigi.brugnano@unifi.it
[4] E-mail: felix@dm.uniba.it
[5] E-mail: trigiant@unifi.it

where J is a skew-symmetric constant matrix, and the Hamiltonian $H(y)$ is assumed to be sufficiently differentiable. For its numerical integration, the problem is to find numerical methods which preserve $H(y)$ along the discrete solution $\{y_n\}$, since this property holds for the continuous solution $y(t)$.

So far, many attempts have been made inside the class of Runge-Kutta methods, the most successful of them being that of imposing the symplecticity of the discrete map, considering that, for the continuous flow, symplecticity implies the conservation of $H(y)$. Concerning symplectic integrators, a backward error analysis permits to prove that they exactly conserve a modified Hamiltonian, even though this fact clearly does not always guarantee a proper qualitative behavior of the discrete orbits.

On the other hand, it is possible to follow different approaches to derive geometric integrators which are energy-preserving. This has been done, for example, in the pioneering work [6], and later in [14], where *discrete gradient methods* are introduced and studied. An additional example of energy-preserving method is the *Averaged Vector Field (AVF)* method defined in [15] (see also [4]). By the way, the latter method can be retrieved by the methods here studied.

More recently, in [2] a new family of one-step methods has been introduced, capable of providing a numerical solution $\{y_n\}$ of (1), along which the energy function $H(y)$ is precisely conserved, in the case where this function is a polynomial (see also [10, 11, 1]).

These methods, named *Hamiltonian Boundary Value Methods* (*HBVMs* hereafter), may be also thought of as Runge-Kutta methods where the internal stages are split into two categories:

- the *fundamental stages*, whose number, say s, is related to the order of the method;
- the *silent stages*, whose number, say r, has to be suitably selected in order to assure the energy conservation property for a polynomial $H(y)$ of given degree ν; the higher is ν, the higher must be r.

The resulting method is denoted by HBVM(k, s),[6] where $k = s + r$ is the total number of *unknown* stages.

In [2, 11] it has also been shown that these new methods provide a practical conservation of the energy even in the non-polynomial case: the term "practical" means that, in many general situations, when the number of silent stages is high enough, the method makes no distinction between the function $H(y)$ and its polynomial approximation, being the latter in a neighborhood of size ε of the former, where ε denotes the machine precision.

Another relevant issue to be mentioned is that the computational cost for the solution of the associated nonlinear system is essentially independent of the number of silent stages, and only depends on s (see [2, 1]). This comes from the fact that the silent stages are actually linear combinations of the fundamental stages.

These two aspects motivate the following question: *what is, if any, the limit method when the number of silent stages grows to infinity?*

This question was first posed by Ernst Hairer,[7] who also provided a partial answer by stating formulae (21), which he called *Energy Preserving variant of Collocation Methods* (*EPCMs*, hereafter) [7]. We provide a proof of his statement by clarifying the connection between the limit formulae and HBVMs: we show that actually one can define several different limit methods,[8] each one associated to the specific polynomial basis, as well as to the choice of the abscissae distribution, used to construct the sequence of HBVMs. For example, EPCMs are based upon the use of Lagrange polynomials, while, working with the shifted Legendre basis, yields to different limit methods, that we have called *Infinity Hamiltonian Boundary Value Methods* (in short, ∞-*HBVMs* or *HBVM*(∞, s), being s the number of the *unknown* fundamental stages).

Our aim in this paper is threefold:

[6] The denomination *HBVM* with k *steps* and *degree* s was used in [2].

[7] During the international conference "ICNAAM 2009", Rethymno, Crete, Greece, 18-22 September 2009, after the talks, by the first two authors, where HBVMs were presented.

[8] In the sense that they generate different discrete problems.

1. We settle the definition of HBVMs in a more general framework, also deriving the general formulation of the limit formulae
$$\lim_{k\to\infty} \text{HBVM}(k,s).$$
In particular, we show that such limit coincides with EPCMs if the Lagrange polynomial basis is used (Section 2).

2. In Section 3, we introduce the new class of ∞-HBVMs, which are the limit formulae corresponding to the HBVMs based upon the shifted Legendre polynomial basis. We prove that the order of such formulae is the same as the Gauss-Legendre methods, that is $2s$ (where s is the number of the unknown fundamental stages).

3. We mention the case where $H(y)$ belongs to vector spaces different from that of polynomials, thus providing a natural (and trivial) generalization of the original formulae (see Section 4). Moreover, in the polynomial case, we determine the *optimal* distribution of the nodes (Section 5).

We stress that any finite approximation of EPCMs or ∞-HBVMs based on quadratures leads back to HBVM(k,s) methods, for k high enough.

We address all the points listed above, by slightly modifying the approach followed to define the class of HBVMs in [2].

2 Reformulation of Hamiltonian BVMs

The key formula which HBVMs rely on, is the *line integral* and the related property of conservative vector fields:
$$H(y_1) - H(y_0) = h\int_0^1 \dot\sigma(t_0+\tau h)^T \nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad \text{for any } y_1 \in \mathbb{R}^{2m}, \tag{2}$$
where σ is any smooth function such that
$$\sigma(t_0) = y_0, \qquad \sigma(t_0+h) = y_1. \tag{3}$$
Here we consider the case where $\sigma(t)$ is a polynomial (of degree at most s), yielding an approximation to the true solution $y(t)$ in the time interval $[t_0, t_0+h]$. The numerical approximation for the subsequent time-step, y_1, is then defined by (3). After introducing a set of s distinct abscissae $c_1,\dots,c_s$, $(0 < c_i \le 1)$,[9] we set
$$Y_i = \sigma(t_0+c_i h), \qquad i = 1,\dots,s, \tag{4}$$
so that $\sigma(t)$ may be thought of as an interpolation polynomial, Y_i, $i=1,\dots,s$, being the internal stages.

Let us consider the following expansions of $\dot\sigma(t)$ and $\sigma(t)$ for $t\in[t_0,t_0+h]$:
$$\dot\sigma(t_0+\tau h) = \sum_{j=1}^s \gamma_j P_j(\tau), \qquad \sigma(t_0+\tau h) = y_0 + h\sum_{j=1}^s \gamma_j \int_0^\tau P_j(x)\,\mathrm{d}x, \tag{5}$$
where $\{P_j(t)\}$ is any suitable basis of the vector space of polynomials of degree at most $s-1$ and the (vector) coefficients $\{\gamma_j\}$ are to be determined.[10] Before proceeding, one important remark is in order.

[9] As a convention, when $c=0$ is to be considered, as in the case of the Lobatto abscissae in $[0,1]$, then $c_0=0$ is formally added to the abscissae $c_1,\dots,c_s$, and the subsequent formulae are modified accordingly.

[10] More general function spaces will be considered in the sequel.

Remark 1. *As will be clear in a while, we observe that the numerical method which the following procedure will define is "basis-dependent", in that to different choices of the basis $\{P_j(t)\}$ there will, in general, correspond different numerical methods. In this section, in order to let the theory be presented as general as possible, we leave the basis not better specified. This will allow us to achieve the results listed at point 1. in the introduction. The question about how to choose the basis properly is faced in Section 3, where ∞-HBVMs will be introduced. Therefore, just in the present section, to avoid confusion, we will always specify what is the basis we are working with. This will be not necessary anymore starting from Section 3, after determining the optimal basis.*

In this section we assume that $H(y)$ is a polynomial, which implies that the integrand in (2) is also a polynomial so that the line integral can be exactly computed by means of a suitable quadrature formula. It is easy to observe that in general, due to the high degree of the integrand function, such quadrature formula cannot be solely based upon the available abscissae $\{c_i\}$: one needs to introduce an additional set of abscissae, $\hat{c}_1, \dots, \hat{c}_r$, distinct from the nodes $\{c_i\}$, in order to make the quadrature formula exact:

$$\begin{aligned}\int_0^1 \dot\sigma(t_0+\tau h)^T \nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau = \\ \sum_{i=1}^s \beta_i \dot\sigma(t_0+c_i h)^T \nabla H(\sigma(t_0+c_i h)) + \sum_{i=1}^r \hat\beta_i \dot\sigma(t_0+\hat c_i h)^T \nabla H(\sigma(t_0+\hat c_i h)),\end{aligned} \tag{6}$$

where β_i, $i = 1, \dots, s$, and $\hat\beta_i$, $i = 1, \dots, r$, denote the weights of the quadrature formula corresponding to the abscissae $\{c_i\}$ and $\{\hat c_i\}$, respectively, i.e.,

$$\begin{aligned}\beta_i &= \int_0^1 \left(\prod_{j=1, j\neq i}^s \frac{t-c_j}{c_i-c_j}\right)\left(\prod_{j=1}^r \frac{t-\hat c_j}{c_i-\hat c_j}\right)\mathrm{d}t, \qquad i=1,\dots,s,\\ \hat\beta_i &= \int_0^1 \left(\prod_{j=1}^s \frac{t-c_j}{\hat c_i-c_j}\right)\left(\prod_{j=1, j\neq i}^r \frac{t-\hat c_j}{\hat c_i-\hat c_j}\right)\mathrm{d}t, \qquad i=1,\dots,r.\end{aligned} \tag{7}$$

According to [11], the right-hand side of (6) is called *discrete line integral*, while the vectors

$$\hat Y_i = \sigma(t_0+\hat c_i h), \qquad i=1,\dots,r, \tag{8}$$

are called *silent stages*: they just serve to increase, as much as one likes, the degree of precision of the quadrature formula, but they are not to be regarded as unknowns since, from (5), they can be expressed in terms of linear combinations of the *fundamental stages* (4).

In [2], the method HBVM(k,s), with $k = s + r$ is then defined by substituting the quantities in (5) into the right-hand side of (6) and by choosing the unknowns $\{\gamma_j\}$ in order that the resulting expression vanishes.

Instead of carrying out our computation on the right-hand side of (6), as was done in [2], we apply the procedure directly to the original line integral appearing in the left-hand side. Of course, since these two expressions are equal, the final formula will exactly match the HBVM(k,s) method, written in a different guise.

With this premise, by considering the first expansion in (5), the conservation property reads

$$\sum_{j=1}^s \gamma_j^T \int_0^1 P_j(\tau)\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau = 0, \tag{9}$$

which, as is easily checked, is certainly satisfied if we impose the following set of orthogonality conditions

$$\gamma_j = \eta_j \int_0^1 P_j(\tau) J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad j=1,\dots,s, \tag{10}$$

with $\{\eta_j\}$ suitably *nonzero* scaling factors that will be defined in a while. Then, from the second relation of (5) we obtain, by introducing the operator

$$\begin{aligned} &L(f;h)\sigma(t_0+ch) = \\ &\qquad \sigma(t_0) + h\sum_{j=1}^{s}\eta_j \int_0^c P_j(x)\mathrm{d}x \int_0^1 P_j(\tau) f(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad c\in[0,1], \end{aligned} \tag{11}$$

that σ is the eigenfunction of $L(J\nabla H;h)$ relative to the eigenvalue $\lambda=1$:

$$\sigma = L(J\nabla H;h)\sigma. \tag{12}$$

Definition 1. *Equation (12) will be called the* Master Functional Equation *defining* σ.

Remark 2. *We also observe that, from (10) and the first relation in (5), one obtains the equations*

$$\dot\sigma(t_0+c_ih) = \sum_{j=1}^{s}\eta_j P_j(c_i)\int_0^1 P_j(\tau)J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad i=1,\dots,s, \tag{13}$$

which may be viewed as extended collocation conditions *according to [11, Section 2], where the integrals are (exactly) replaced by discrete sums (see, e.g., (6)–(7)).*

To practically compute σ, we set (see (4) and (5))

$$Y_i = \sigma(t_0+c_ih) = y_0 + h\sum_{j=1}^{s} a_{ij}\gamma_j, \qquad i=1,\dots,s, \tag{14}$$

where

$$a_{ij} = \int_0^{c_i} P_j(x)\mathrm{d}x, \qquad i,j=1,\dots,s. \tag{15}$$

Inserting (10) into (14) yields the final formulae which define the HBVMs class based upon the basis $\{P_j\}$:

$$Y_i = y_0 + h\int_0^1 \left(\sum_{j=1}^{s}\eta_j a_{ij}P_j(\tau)\right) J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau, \qquad i=1,\dots,s. \tag{16}$$

The constants $\{\eta_j\}$ have to be chosen in order to make the formula consistent. Problem (14)–(16) can be actually solved, provided that all the $\{\eta_j\}$ are different from zero,[11] and the matrix

$$\begin{pmatrix} \int_0^{c_1} P_1(x)\mathrm{d}x & \dots & \int_0^{c_s} P_1(x)\mathrm{d}x \\ \vdots & & \vdots \\ \int_0^{c_1} P_s(x)\mathrm{d}x & \dots & \int_0^{c_s} P_s(x)\mathrm{d}x \end{pmatrix}$$

is nonsingular (which we shall obviously assume hereafter). Indeed, such a matrix allows us, by using (5), to reformulate equation (16) in terms of the (unknown) fundamental stages (4). Let us now formally set

$$f(y) = J\nabla H(y), \tag{17}$$

and report a few examples for possible choices of the basis $\{P_j(x)\}$.

[11] For example, the choice $P_j(x) = x^{j-1}$, $j=1,\dots,s$, would lead to $\eta_1=1$, and $\eta_j=0$, $j=2,\dots,s$. This implies that, with this choice of the basis, σ can only be a line (i.e., $s=1$).

1. In [11] we have chosen $\{P_1(x), \ldots, P_s(x)\}$ as the Newton basis. This has allowed us the construction of a family of methods of order 2 and 4.

2. In [2], the abscissae $\{c_0 = 0\} \cup \{c_i\} \cup \{\hat{c}_i\}$ are disposed according to a Lobatto distribution with $k+1$ points in $[0,1]$ and $\{P_1(x), \ldots, P_s(x)\}$ is the shifted Legendre basis in the interval $[0,1]$.[12] Consequently, choosing in (16) $t_0 = 0, h = 1$, and $f(y(\tau)) = P_j(\tau)$, the consistency condition yields
$$\eta_j = \left(\int_0^1 P_j^2(x) \mathrm{d}x \right)^{-1} = 2j - 1, \quad j = 1, \ldots, s, \tag{18}$$
which is exactly the value found in [2]. In such a case, it has been shown that the resulting method has order $2s$, just the same as the generating Lobatto IIIA method (obtained for $k = s$).

3. In a similar way, when using the Lagrange basis $\{\ell_j(x)\}$, by setting $f(y(\tau)) \equiv 1$, one obtains $\eta_j = 1/b_j$ with
$$b_j = \int_0^1 \ell_j(x) \mathrm{d}x, \qquad \ell_j(x) = \prod_{i=1,\, i\neq j}^{s} \frac{x - c_i}{c_j - c_i}. \tag{19}$$
Consequently, formulae (16) become
$$Y_i = y_0 + h \int_0^1 \left(\sum_{j=1}^{s} \frac{a_{ij}}{b_j} \ell_j(\tau) \right) J \nabla H(\sigma(t_0 + \tau h)) \mathrm{d}\tau, \qquad i = 1, \ldots, s. \tag{20}$$
Moreover, by introducing the new variables $K_i = \dot{\sigma}(t_0 + c_i h)$, which are therefore related to the Y_i as
$$Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} K_j, \qquad i = 1, \ldots, s,$$
system (20) can be recast in the equivalent form provided by the *extended collocation conditions* (13):
$$K_i = \frac{1}{b_i} \int_0^1 \ell_i(\tau) J \nabla H(\sigma(t_0 + \tau h)) \mathrm{d}\tau, \qquad i = 1, \ldots, s. \tag{21}$$

Formulae (21) are the ones E. Hairer proposed in the general case, that is for any kind of Hamiltonian function. They were called *Energy Preserving variant of Collocation Methods* (EPCMs) [7]. The above discussion then proves that if the integral can be substituted by a finite sum, as in the case where $H(y)$ is a polynomial, formulae (16), and consequently (21), become a HBVM(k,s), with a suitable value of k.[13]

For sake of completeness, we report the nonlinear system associated with the HBVM(k,s) method, in terms of the fundamental stages $\{Y_i\}$ and the silent stages $\{\hat{Y}_i\}$ (see (8)), by using the notation (17). In this context, they represent the discrete counterpart of (16), and may be directly retrieved by evaluating, for example, the integrals in (16) by means of the (exact) quadrature formula introduced in (6):
$$\begin{aligned} Y_i &= y_0 + h \left[\sum_{l=1}^{s} \beta_l \left(\sum_{j=1}^{s} \eta_j a_{ij} P_j(c_l) \right) f(Y_l) + \sum_{l=1}^{r} \hat{\beta}_l \left(\sum_{j=1}^{s} \eta_j a_{ij} P_j(\hat{c}_l) \right) f(\widehat{Y}_l) \right] \\ &= y_0 + h \sum_{j=1}^{s} \eta_j a_{ij} \left(\sum_{l=1}^{s} \beta_l P_j(c_l) f(Y_l) + \sum_{l=1}^{r} \hat{\beta}_l P_j(\hat{c}_l) f(\widehat{Y}_l) \right), \qquad i = 1, \ldots, s. \end{aligned} \tag{22}$$

[12] More precisely, $P_j(x)$ is here the shifted Legendre polynomial of degree $j-1$, $j = 1, \ldots, s$.
[13] The same clearly happens when the integral is only *approximated* by a finite sum.

From the above discussion it is clear that, in the non-polynomial case, supposing to choose the abscissae $\{\hat{c}_i\}$ so that the sums in (22) converge to an integral as $r = k-s \to \infty$, the resulting formula is (16).[14] Consequently, EPCMs may be viewed as the limit of HBVMs family, when the Lagrange basis is considered, as the number of silent stages grows to infinity.

The above arguments also imply that HBVMs may be as well applied in the non-polynomial case since, in finite precision arithmetic, HBVMs are indistinguishable from their limit formulae (16), when a sufficient number of silent stages is introduced. The aspect of having a *practical* exact integral, for k large enough, was already stressed in [2, 10, 11].

3 Infinity Hamiltonian Boundary Value Methods

As is easily argued (and emphasized in Remark 1), the choice of the basis along which $\dot\sigma(t_0+\tau h)$ is expanded (see (5)), somehow influences the shape of the final formulae (16), that is, to two different polynomial bases there may correspond two different families of formulae.[15] The question then naturally arises about the best possible choice of the basis to consider. This issue has been a crucial point in devising the class of HBVMs in [2] and deserves a particular attention.[16]

Indeed, we recall that our final goal is to devise methods that make the sum (9), representing the line integral, vanish. This is accomplished by the orthogonality conditions (10), whose effect is to make null each term of the sum in (9). It follows that such conditions are in general too demanding, in that they are sufficient but not necessary to get conservativeness. In fact, the sum could in principle vanish even in the case when two ore more of its terms are different from zero. This *extra constraint* may affect the general properties of the conservative methods we are interested in, and in particular their order.

This was a problem already encountered in [11] where the authors realized that the use of the Newton basis didn't assure the expected growth of the order of the resulting method when the degree of the polynomial $\sigma(t_0+\tau h)$ was increased. This barrier has been definitively overcome in [2], where it was understood that the proper polynomial basis to be used by default was that of the shifted Legendre polynomials in the interval $[0,1]$. We emphasize that, contrary to what happens for the Lagrange and Newton bases, the Legendre polynomials are orthogonal and symmetric in the interval $[0,1]$ and in addition they are *abscissae-free*, that is they by no means depend on the specific distribution of the abscissae $\{c_i\}$ adopted. This, in turn, implies that the *Master Functional Equation* (12) is independent of the choice of both the abscissae $\{c_i\}$ and $\{\hat{c}_i\}$: the only requirement being that (6) holds true.[17]

From the above arguments, it is clear that the orthogonality conditions (10), i.e., the fulfillment of the *Master Functional Equation* (12), is only a sufficient condition for the conservation property (9) to hold. Such a condition becomes also necessary, when the basis $\{P_j\}$ is orthogonal.

Theorem 1. *Let $\{P_j\}$ be an orthogonal basis on the interval $[0,1]$. Then, assuming $H(y)$ to be suitably differentiable, (9) implies that each term in the sum has to vanish.*

Proof Let us consider, for simplicity, the case of an orthonormal basis, and the expansion

$$g(\tau) \equiv \nabla H(\sigma(t_0+\tau h)) = \sum_{\ell\ge 1} \rho_\ell P_\ell(\tau), \qquad \rho_\ell = (P_\ell, g), \qquad \ell \ge 1,$$

where, in general,

$$(f,g) = \int_0^1 f(\tau) g(\tau) \mathrm{d}\tau.$$

[14] This obvious requirement for the abscissae will be always assumed in the sequel.
[15] For example, see the method presented in subsection 4.2.
[16] The argument presented here is the analog of the one appearing in [11, Remark 3.1].
[17] We emphasize that this is not the case when using, for example, the Lagrange basis.

Substituting into (9), yields

$$\sum_{j=1}^{s}\gamma_j^T(P_j,g)=\sum_{j=1}^{s}\gamma_j^T\left(P_j,\sum_{\ell\geq 1}\rho_\ell P_\ell\right)=\sum_{j=1}^{s}\gamma_j^T\rho_j=0.$$

Since this has to hold whatever the choice of the function $H(y)$, one concludes that

$$\gamma_j^T\rho_j=0,\qquad j=1,\ldots,s.\ \square \tag{23}$$

Remark 3. *In the case where $\{P_j\}$ is the shifted Legendre basis, from (23) one derives that*

$$\gamma_j=S\rho_j,\qquad i=1,\ldots,s,$$

where S is any nonsingular skew-symmetric matrix. The natural choice $S=J$ then leads to (10), with $\eta_j=(P_j,P_j)^{-1}=2j-1$.

The use of the Legendre basis allows the resulting methods to have the best order and stability properties that one can expect. This aspect is elucidated in the two theorems and the corollary below, which represent the main result of the present work.

Although, up to now, we have maintained the treatment of HBVMs at a general level, it is clear that, in view of the result presented in Theorem 2, when the curve $\sigma(t_0+\tau h)$ is assumed of polynomial type, we will implicitly adopt the Legendre basis.[18] This important assumption will be incorporated in the HBVM methods from now on: if needed, the use of any other kind of basis will be explicitly stated, in order not to create confusion.

Taking into account the consistency conditions (18), formula (16)–(15) takes the form:

$$Y_i=y_0+h\int_0^1\left(\sum_{j=1}^{s}(2j-1)a_{ij}P_j(\tau)\right)J\nabla H(\sigma(t_0+\tau h))\mathrm{d}\tau,\qquad i=1,\ldots,s. \tag{24}$$

If the Hamiltonian $H(y)$ is a polynomial, the integral appearing at the right-hand side is exactly computed by a quadrature formula, thus resulting into a HBVM(k,s) method with a sufficient number of silent stages. As already stressed in the previous section, in the non-polynomial case such formulae represent the limit of the sequence HBVM(k,s), as $k\to\infty$.

Definition 2. *We call the new limit formula (24) an* Infinity Hamiltonian Boundary Value Method *(in short, ∞-HBVM or HBVM(∞,s)).*

We emphasize that, in the non-polynomial case, (24) becomes an operative method, only after that a suitable strategy to approximate the integral is taken into account (see the next section for additional examples). In the present case, if one discretizes the *Master Functional Equation* (11)–(12), HBVM(k,s) are then obtained, essentially by extending the discrete problem (22) also to the silent stages (8). In order to simplify the exposition, we shall use (17) and introduce the following notation:

$$\{t_i\}=\{c_i\}\cup\{\hat c_i\},\quad \{\omega_i\}=\{\beta_i\}\cup\{\hat\beta_i\},\quad y_i=\sigma(t_0+t_ih),\quad f_i=f(\sigma(t_0+t_ih)). \tag{25}$$

The discrete problem defining the HBVM(k,s) then becomes, with $\eta_j=2j-1$,

$$y_i=y_0+h\sum_{j=1}^{s}\eta_j\int_0^{t_i}P_j(x)\mathrm{d}x\sum_{\ell=1}^{k}\omega_\ell P_j(t_\ell)f_\ell,\qquad i=1,\ldots,k. \tag{26}$$

[18] Actually, the term *Hamiltonian Boundary Value Method* has been coined in [2], after introducing the Legendre basis.

We can cast the set of equations in vector form, by introducing the vectors $\boldsymbol{y} = (y_1^T, \ldots, y_k^T)^T$, $e = (1, \ldots, 1)^T \in \mathbb{R}^k$, and the matrices $\mathcal{I}, \mathcal{P} \in \mathbb{R}^{k \times s}$, with

$$\mathcal{I}_{ij} = \int_0^{t_i} P_j(x)\mathrm{d}x, \quad \mathcal{P}_{ij} = P_j(t_i), \quad \text{and} \quad \Lambda = \mathrm{diag}(\eta_1, \ldots, \eta_s), \quad \Omega = \mathrm{diag}(\omega_1, \ldots, \omega_k), \tag{27}$$

as

$$\boldsymbol{y} = e \otimes y_0 + h(\mathcal{I}\Lambda\mathcal{P}^T\Omega) \otimes I\, f(\boldsymbol{y}), \tag{28}$$

with an obvious meaning of $f(\boldsymbol{y})$. Consequently, the method can be seen as a Runge-Kutta method with the following Butcher tableau:

$$\begin{array}{c|c} t_1 & \\ \vdots & \mathcal{I}\Lambda\mathcal{P}^T\Omega \\ t_k & \\ \hline & \omega_1 \ \ldots \ \omega_k \end{array} \tag{29}$$

Remark 4. *We observe that, provided that the matrix Λ is independent of the basic abscissae $\{c_i\}$ (as in the case of the Legendre basis), the role of such abscissae and of the silent abscissae $\{\hat{c}_i\}$ is interchangeable. This is not true, for example, for the Newton and Lagrange bases.*

The following result then holds true.

Theorem 2. *Provided that the quadrature has order at least $2s$ (i.e., it is exact for polynomials of degree at least $2s-1$), HBVM(k,s) has order $p = 2s \equiv 2\deg(\sigma)$, whatever the choice of the abscissae $c_1, \ldots, c_s$.*

Proof From the classical result of Butcher (see, e.g., [9, Theorem 7.4]), the thesis follows if the simplifying assumptions $C(s)$, $B(p)$, $p \geq 2s$, and $D(s-1)$ are satisfied. By looking at the method (28)–(29), one has that the first two (i.e., $C(s)$ and $B(p)$, $p \geq 2s$) are obviously fulfilled: the former by the definition of the method, the second by hypothesis. The proof is then completed, if we prove $D(s-1)$. Such condition can be cast in matrix form, by introducing the vector $\bar{e} = (1, \ldots, 1)^T \in \mathbb{R}^{s-1}$, and the matrices

$$Q = \mathrm{diag}(1, \ldots, s-1), \qquad D = \mathrm{diag}(t_1, \ldots, t_k), \qquad V = (t_i^{j-1}) \in \mathbb{R}^{k \times s-1},$$

(see also (27)) as

$$QV^T\Omega\left(\mathcal{I}\Lambda\mathcal{P}^T\Omega\right) = \left(\bar{e}\, e^T - V^T D\right)\Omega,$$

i.e.,

$$\mathcal{P}\Lambda\mathcal{I}^T\Omega V Q = \left(e\, \bar{e}^T - DV\right). \tag{30}$$

Since the quadrature is exact for polynomial of degree $2s-1$. one has

$$\begin{aligned} \left(\mathcal{I}^T\Omega V Q\right)_{ij} &= \left(\sum_{\ell=1}^{k} \omega_\ell \int_0^{t_\ell} P_i(x)\mathrm{d}x\, (jt_\ell^{j-1})\right) = \left(\int_0^1 \int_0^t P_i(x)\mathrm{d}x (jt^{j-1})\mathrm{d}t\right) \\ &= \left(\delta_{i1} - \int_0^1 P_i(x)x^j\mathrm{d}x\right), \qquad i = 1, \ldots, s, \quad j = 1, \ldots, s-1, \end{aligned}$$

where the last equality is obtained by integrating by parts, with δ_{i1} the Kronecker symbol. Consequently,

$$\left(\mathcal{P}\Lambda\mathcal{I}^T\Omega V Q\right)_{ij} = \left(1 - \sum_{\ell=1}^{s} \eta_\ell P_\ell(t_i) \int_0^1 P_\ell(x)x^j\mathrm{d}x\right) = (1 - t_i^j), \quad i = 1, \ldots, k, \quad j = 1, \ldots, s-1,$$

that is, (30), where the last equality follows from the fact that

$$\sum_{\ell=1}^{s} \eta_\ell P_\ell(t) \int_0^1 P_\ell(x) x^j \mathrm{d}x = t^j, \qquad j = 1, \ldots, s-1. \,\square$$

Concerning the stability, the following result holds true.

Theorem 3. *For all k such that the quadrature formula has order at least $2s \equiv 2\deg(\sigma)$, HBVM(k,s) is perfectly A-stable, whatever the choice of the abscissae $c_1, \ldots, c_s$.*

Proof As it has been previously observed, a HBVM(k, s) is fully characterized by the corresponding polynomial σ which, for k sufficiently large (i.e., assuming that (6) holds true), satisfies the *Master Functional Equation* (11)–(12), which is independent of the choice of the nodes $c_1, \ldots, c_s$ (since we consider the Legendre basis). When, in place of $f(y) = J\nabla H(y)$ we put the test equation $f(y) = \lambda y$, we have that the collocation polynomial of the Gauss-Legendre method of order $2s$, say σ_s, satisfies the *Master Functional Equation*, since the integrands appearing in it are polynomials of degree at most $2s-1$, so that $\sigma = \sigma_s$. The proof completes by considering that Gauss-Legendre methods are perfectly A-stable. $\square$

A worthwhile consequence of Theorems 2 and 3 is that one can transfer to HBVM(∞, s) all those properties of HBVM(*k*,*s*) which are satisfied starting from a given $k \geq k_0$ on: for example, the order and stability properties.

Corollary 1. *Whatever the choice of the abscissae $c_1, \ldots, c_s$, HBVM(∞, s)* (24) *has order $2s$ and is perfectly A-stable.*

Remark 5. *From the result of Corollary 1, it follows that HBVM(∞, s) has order $2s$ and is perfectly A-stable for* any *choice for the abscissae $c_1, \ldots, c_s$. Since such abscissae can be arbitrarily chosen, we can formally place them at the roots of the Gauss-Legendre polynomial of degree s. On the other hand, by considering that, at such abscissae, by setting $\{\ell_i(c)\}$ and $\{b_i\}$ the corresponding Lagrange polynomials and quadrature weights, respectively (see (19)),*

$$\frac{1}{b_i} \int_0^1 P_j(x)\ell_i(x)\mathrm{d}x = \frac{1}{b_i} \sum_{r=1}^{s} b_r P_j(c_r)\ell_i(c_r) = P_j(c_i), \qquad j = 1, \ldots, s,$$

one obtains (with $\eta_j = 2j-1$ and by using the notation (17)):

$$\begin{aligned}
\sigma'(t_0 + c_i h) &= \sum_{j=1}^{s} \eta_j P_j(c_i) \int_0^1 P_j(\tau) f(\sigma(t_0 + \tau h))\mathrm{d}\tau \\
&= \sum_{j=1}^{s} \eta_j \left(\frac{1}{b_i} \int_0^1 P_j(x)\ell_i(x)\mathrm{d}x \right) \int_0^1 P_j(\tau) f(\sigma(t_0 + \tau h))\mathrm{d}\tau \\
&= \frac{1}{b_i} \int_0^1 \left(\sum_{j=1}^{s} \eta_j P_j(\tau) \int_0^1 P_j(x)\ell_i(x)\mathrm{d}x \right) f(\sigma(t_0 + \tau h))\mathrm{d}\tau \\
&= \frac{1}{b_i} \int_0^1 \ell_i(\tau) f(\sigma(t_0 + \tau h))\mathrm{d}\tau, \qquad i = 1, \ldots, s.
\end{aligned}$$

Consequently, for any choice of the abscissae $\{c_i\}$, *HBVM(∞, s) provide the same polynomial σ as the "optimal EPCMs" (21) of order $2s$ [7].*[19] *Conversely, an EPCM is optimal (i.e., it has order $2s$)* only *when*

[19] In this sense, they are *equivalent*, even though they generate different discrete problems.

the abscissae $c_1, \dots, c_s$ define a quadrature formula of order at least $2s-1$, whereas different choices result in methods of lower order [7, Theorem 1].

Remark 6. *We also observe that, due to the choice of the shifted Legendre polynomial basis (see (24))*

$$\textit{HBVM}(\infty, s) = \lim_{k\to\infty} \textit{HBVM}(k, s),$$

whatever is the choice of the fundamental abscissae $\{c_i\}$. Consequently, for all k large enough, so that the Master Functional Equation *(12) holds true (e.g., in the case of a polynomial Hamiltonian $H(y)$), all HBVM(k,s) provide the same polynomial σ of degree s,* independently of the choice of the abscissae $\{c_i\}$. *Hence, they are* equivalent *to each other. This result doesn't change in the case where $H(y)$ is not a polynomial, provided that $H(y)$ is sufficiently differentiable. In this case, in fact, one formally obtains, in place of the* Master Functional Equation (12)*, an equation of the form*

$$\sigma_k = L(J\nabla H; h)\sigma_k + \psi_k(h), \tag{31}$$

where $\psi_k(h) = O(h^{q_k-s+2})$, q_k being the degree of precision of the quadrature at the right-hand side in (6), so that $q_k \to \infty$ as $k \to \infty$. From (12) and (31), one then obtains that as $h \to 0$, assuming that f is Lipschitzian with constant μ, and for a suitable constant M independent of h:

$$\|\sigma_k - \sigma\| \le h\mu M\|\sigma_k - \sigma\| + \|\psi_k(h)\|,$$

i.e.,

$$\|\sigma_k - \sigma\| \le (1 - h\mu M)^{-1}\|\psi_k(h)\| = O(h^{q_k-s+2}) \to 0, \qquad k \to \infty.$$

One then concludes that, when using finite precision arithmetic, σ_k is indistinguishable from σ, for all k large enough.

Example 1. *As previously mentioned, for the methods studied in [2], based on a Lobatto distribution of the nodes $\{c_0 = 0, c_1, \dots, c_s\} \cup \{\hat c_1, \dots, \hat c_{k-s}\}$, one has that $\deg(\sigma) = s$, so that the order of HBVM(k,s) turns out to be $2s$, with a quadrature satisfying $B(2k)$.*

Example 2. *For the same reason, when one considers a Gauss distribution for the abscissae $\{c_1, \dots, c_s\} \cup \{\hat c_1, \dots, \hat c_{k-s}\}$, one also obtains a method of order $2s$ with a quadrature satisfying $B(2k)$. This case will be further studied in Section 5.*

Remark 7. *Finally, we also mention that, from Remark 4, HBVM(k,s) are symmetric methods,*[20] *provided that the abscissae $\{t_i\}$ (see (25)) are symmetrically distributed (see also [2]).*

4 Generalization of Hamiltonian BVMs

The approach that has allowed the construction of methods that conserve energy functions of polynomial type is quite general: that is, by no means it depends on the particular vector space generating the curve $\sigma(t)$ nor on the quadrature technique used. As was emphasized in [11, Section 2], it solely relies on the following two ingredients: the definition of *discrete line integral* and the *extended collocation conditions* (13), which zero the line integral (6).

Therefore, in a more general context, this procedure can be formalized as follows. One first picks a curve $\sigma(t_0 + \tau h)$, $\tau \in [0, 1]$, joining two points of the phase space $y_0 = \sigma(t_0)$ and $y_1 = \sigma(t_0 + h)$. Such a curve is assumed to lie in a proper finite dimensional vector space $W = \mathrm{span}\{P_1(x), \dots, P_s(x)\}$, where now $P_j(x)$, $j = 1, \dots, s$, are any linearly independent functions. Therefore the curves $\sigma(t)$ and $\dot\sigma(t)$ will admit an expansion in the form (5).

[20] According to the *time reversal symmetry condition* defined in [3, p. 218].

The fundamental hypothesis, for this approach to work, is that the choice of W must guarantee that the functions $P_j(\tau)\nabla H(\sigma(t_0+\tau h))$ appearing in (9) (and hence $\dot\sigma(t)^T\nabla H(\sigma(t))$) be elementary integrable, that is they are required to admit a primitive that can be expressed in terms of elementary functions. If this is the case, all the steps performed to obtain (16) may be repeated with the integral substituted by the primitive.

This represents a generalization of what done for polynomial Hamiltonian functions not only because the vector space W may be generated by non-polynomial functions but also because the analytic solution of the line integral may be carried out by any available technique. Hereafter, we report a couple of examples in the class (24).[21]

4.1 A method of order two

We consider a separable Hamiltonian function (for simplicity we assume $m = 1$)

$$H(q,p) = V(p) - U(q). \tag{32}$$

Let $\sigma(t)$ be the segment joining $y_0 = (q_0,p_0)^T$ to $y_1 = (q_1,p_1)^T$:

$$\sigma(t_0+\tau h) = y_0 + \tau(y_1 - y_0).$$

We have $c_0 = 0$, $c_1 = 1$, and the corresponding method (24) becomes:

$$\begin{pmatrix} \dfrac{q_1-q_0}{h} \\ \dfrac{p_1-p_0}{h} \end{pmatrix} = \begin{pmatrix} \displaystyle\int_0^1 V'(p_0+\tau(p_1-p_0))\mathrm{d}\tau \\ \displaystyle\int_0^1 U'(q_0+\tau(q_1-q_0))\mathrm{d}\tau \end{pmatrix} = \begin{pmatrix} \dfrac{V(p_1)-V(p_0)}{p_1-p_0} \\ \dfrac{U(q_1)-U(q_0)}{q_1-q_0} \end{pmatrix}. \tag{33}$$

Formula (33) is one of the simplest *discrete gradient methods* due to Itoh and Abe [12], whose general form, for non-separable Hamiltonian functions with one degree of freedom, reads

$$\begin{pmatrix} \dfrac{q_1-q_0}{h} \\ \dfrac{p_1-p_0}{h} \end{pmatrix} = J \begin{pmatrix} \dfrac{H(q_1,p_0)-H(q_0,p_0)}{q_1-q_0} \\ \dfrac{H(q_1,p_1)-H(q_1,p_0)}{p_1-p_0} \end{pmatrix}. \tag{34}$$

The vector appearing at the right-hand side of (34) is obtained by replacing the partial derivatives of $H(q,p)$ with increments along the q and p axes. Method (34) is in general first order and nonsymmetric. However, when confined to separable Hamiltonian systems, it turns out to be second order and symmetric.[22]

4.2 A method of order four

To construct a method of order four in the form (24) applied to (32), we pick a curve $\sigma(t)$ of degree two, based upon the abscissae $c_0 = 0$, $c_1 = 1/2$, and $c_2 = 1$. Such a method has been already described in [11] for polynomial Hamiltonian functions: here we consider its generalization to the non-polynomial case. Setting $Y_1 = (q_{1/2},p_{1/2})^T$ and, observing that $Y_2 = (q_1,p_1)^T$, the two components of the curve $\sigma(t_0+\tau h)$ are

$$\begin{pmatrix} \sigma_1(t_0+\tau h) \\ \sigma_2(t_0+\tau h) \end{pmatrix} = \begin{pmatrix} 2(q_0-2q_{1/2}+q_1)\tau^2 - (3q_0-4q_{1/2}+q_1)\tau + q_0 \\ 2(p_0-2p_{1/2}+p_1)\tau^2 - (3p_0-4p_{1/2}+p_1)\tau + p_0 \end{pmatrix}. \tag{35}$$

[21] While the method in Section 4.1 is equivalently obtainable by applying either (24) or (16), the same is not true for the fourth-order method derived in Section 4.2 where, the use of the Lagrange basis, would produce a coefficient $b_2 = 0$ (appearing as a denominator in the resulting formulae (21)).

[22] A generalization of (34) introduced in [13] also becomes method (33) when applied to Hamiltonian functions in the form (32).

Consequently, (24) becomes

$$
\begin{aligned}
Y_1 \equiv \begin{pmatrix} q_{1/2} \\ \\ p_{1/2} \end{pmatrix} &= \begin{pmatrix} q_0 \\ \\ p_0 \end{pmatrix} + h \begin{pmatrix} \int_0^1 (-\frac{3}{2}\tau + \frac{5}{4}) V'(\sigma_2(t_0+\tau h))\mathrm{d}\tau \\ \\ \int_0^1 (-\frac{3}{2}\tau + \frac{5}{4}) U'(\sigma_1(t_0+\tau h))\mathrm{d}\tau \end{pmatrix}, \\
Y_2 \equiv \begin{pmatrix} q_1 \\ \\ p_1 \end{pmatrix} &= \begin{pmatrix} q_0 \\ \\ p_0 \end{pmatrix} + h \begin{pmatrix} \int_0^1 V'(\sigma_2(t_0+\tau h))\mathrm{d}\tau \\ \\ \int_0^1 U'(\sigma_1(t_0+\tau h))\mathrm{d}\tau \end{pmatrix}.
\end{aligned}
\tag{36}
$$

Substituting (35) into (36) we obtain a system in the unknowns $q_{1/2}$, $p_{1/2}$, q_1, p_1. Looking at (36), we realize that even in the simpler case of a system deriving from a Hamiltonian function in the form (32), the elementary integrability of the integrals in (24) is not a priori guaranteed. This means that, in this case, we cannot arrive at a general formula analogous to (33), in terms of $U(q)$ and $V(p)$.

On the other hand, in several cases of interest, such primitive can be explicitly computed: hereafter we report a significant example, which we shall use later in the numerical tests in Section 5.

Example 3. The role of this example is also to show that, when finite precision arithmetic is used, it may be *not convenient* to use the *infinite version* of the methods, even if the integrals can be analytically evaluated. This will be evident from the numerical results in Section 5.4. The system we consider is the one defined by the Hamiltonian function

$$H(q,p) = a(\log q - q) + b(\log p - p), \tag{37}$$

where a and b are positive constants. The associated system (1) reads

$$\dot{q} = \quad b\left(\frac{1}{p} - 1\right), \qquad \dot{p} = -a\left(\frac{1}{q} - 1\right). \tag{38}$$

This system is strictly related to the Lotka-Volterra model

$$\begin{cases} \dot{q} = \quad b\,q\,(1-p), \\ \dot{p} = -a\,p\,(1-q), \end{cases} \tag{39}$$

in that system (39) may be recast as the Poisson system $\dot{y} = \frac{1}{\eta(q,p)} J \nabla H(y)$, where $\eta(q,p) = -\frac{1}{qp}$ is called *integrating factor*.

Systems (39) and (38) share the same Hamiltonian function (37) as first integral and, consequently, they share the same curves as trajectories in the phase plane. Method (36) applied to (39) reads

$$
\begin{pmatrix} \frac{q_{1/2}-q_0}{h/2} \\ \\ \frac{p_{1/2}-p_0}{h/2} \end{pmatrix} = \begin{pmatrix} -b + \frac{3}{4} b \frac{\log(|p_0/p_1|)}{p_0 - 2p_{1/2} + p_1} + \frac{1}{2}\frac{b}{C_1}\frac{p_0 - 8p_{1/2} + 7p_1}{p_0 - 2p_{1/2} + p_1} \\ \cdot \left(\operatorname{arctanh}(\frac{-3p_0 + 4p_{1/2} - p_1}{C_1}) - \operatorname{arctanh}(\frac{p_0 - 4p_{1/2} + 3p_1}{C_1})\right) \\ \\ a - \frac{3}{4} a \frac{\log(|q_0/q_1|)}{q_0 - 2q_{1/2} + q_1} - \frac{1}{2}\frac{a}{C_2}\frac{q_0 - 8q_{1/2} + 7q_1}{q_0 - 2q_{1/2} + q_1} \\ \cdot \left(\operatorname{arctanh}(\frac{-3q_0 + 4q_{1/2} - q_1}{C_2}) - \operatorname{arctanh}(\frac{q_0 - 4q_{1/2} + 3q_1}{C_2})\right) \end{pmatrix}, \tag{40}
$$

$$
\begin{pmatrix} \frac{q_1-q_0}{h} \\ \\ \frac{p_1-p_0}{h} \end{pmatrix} = \begin{pmatrix} -b - \frac{2b}{C_1}\left[\operatorname{arctanh}(\frac{p_0 - 4p_{1/2} + 3p_1}{C_1}) + \operatorname{arctanh}(\frac{3p_0 - 4p_{1/2} + p_1}{C_1})\right] \\ \\ a + \frac{2a}{C_2}\left[\operatorname{arctanh}(\frac{q_0 - 4q_{1/2} + 3q_1}{C_2}) + \operatorname{arctanh}(\frac{3q_0 - 4q_{1/2} + q_1}{C_2})\right] \end{pmatrix}, \tag{41}
$$

where

$$\begin{cases} C_1 = (p_0^2 + 16p_{1/2}^2 + p_1^2 - 8p_0p_{1/2} - 2p_0p_1 - 8p_{1/2}p_1)^{1/2}, \\ C_2 = (q_0^2 + 16q_{1/2}^2 + q_1^2 - 8q_0q_{1/2} - 2q_0q_1 - 8q_{1/2}q_1)^{1/2}. \end{cases}$$

5 HBVMs based upon Gauss quadrature

As anticipated in Example 2, we now study the properties of the HBVM(k,s) which is defined over the set of k distinct abscissae,

$$\{t_1,\ldots,t_k\} \equiv \{c_1,\ldots,c_s\} \cup \{\hat{c}_1,\ldots,\hat{c}_{k-s}\},$$

coinciding with the Gauss-Legendre nodes in $[0,1]$, i.e., the roots of the shifted Legendre polynomial of degree k. The corresponding polynomial σ has then degree s. By virtue of Theorems 2 and 3 (see also Remark 7), such methods are symmetric, perfectly A-stable, and of order $2s$. They reduce to Gauss-Legendre collocation methods, when $k = s$, and are exact for polynomial Hamiltonian functions of degree ν, provided that

$$k \geq \frac{\nu s}{2}. \tag{42}$$

By recalling what stated in Remark 6, for all k sufficiently large so that (6) holds, HBVM(k,s) based on the k Gauss-Legendre abscissae in $[0,1]$ are *equivalent* to HBVM(k,s) based on $k+1$ Lobatto abscissae in $[0,1]$ (see [2]), since both methods define the same polynomial σ of degree s.[23]

As matter of fact, we have run HBVM(k,s) based on Gauss-Legendre nodes, and HBVM(k,s) based on the Lobatto nodes, obtaining the same results on the polynomial test problems reported in [2], which are briefly recalled in the sequel.

5.1 Test problem 1

Let us consider the problem characterized by the polynomial Hamiltonian (4.1) in [5],

$$H(p,q) = \frac{p^3}{3} - \frac{p}{2} + \frac{q^6}{30} + \frac{q^4}{4} - \frac{q^3}{3} + \frac{1}{6}, \tag{43}$$

having degree $\nu = 6$, starting at the initial point $y_0 \equiv (q(0),p(0))^T = (0,1)^T$, so that $H(y_0) = 0$. For such a problem, in [5] it has been experienced a numerical drift in the discrete Hamiltonian, when using the fourth-order Lobatto IIIA method with stepsize $h = 0.16$, as confirmed by the plot in Figure 1. When using the fourth-order Gauss-Legendre method the drift disappears, even though the Hamiltonian is not exactly preserved along the discrete solution, as is shown by the plot in Figure 2. On the other hand, by using the fourth-order HBVM(6,2) with the same stepsize, the Hamiltonian turns out to be preserved up to machine precision, as shown in Figure 3, since such method exactly preserves polynomial Hamiltonians of degree up to 6. In such a case, the numerical solutions obtained by using the Lobatto nodes $\{c_0 = 0, c_1, \ldots, c_6 = 1\}$ or the Gauss-Legendre nodes $\{c_1,\ldots,c_6\}$ are the same.

5.2 Test problem 2

The second test problem, having a highly oscillating solution, is the Fermi-Pasta-Ulam problem (see [8, Section I.5.1]), defined by the Hamiltonian

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{m}\left(p_{2i-1}^2 + p_{2i}^2\right) + \frac{\omega^2}{4}\sum_{i=1}^{m}\left(q_{2i} - q_{2i-1}\right)^2 + \sum_{i=0}^{m}\left(q_{2i+1} - q_{2i}\right)^4, \tag{44}$$

[23] In the non-polynomial case, they converge to the same HBVM(∞,s), as $k \to \infty$.

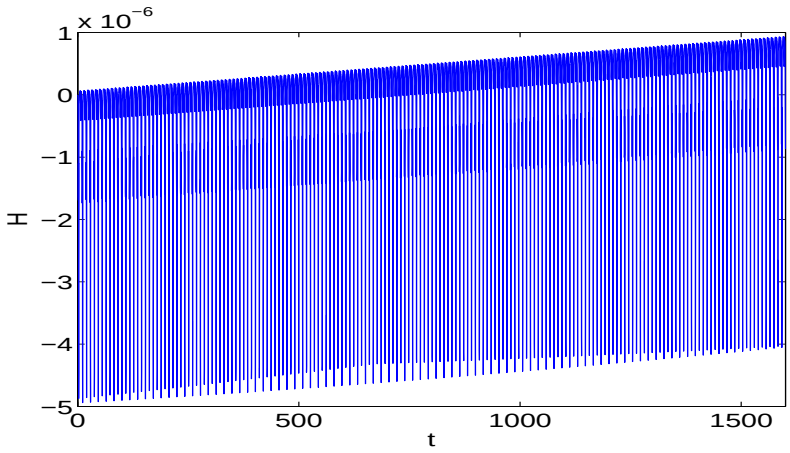

Figure 1: Fourth-order Lobatto IIIA method, $h = 0.16$, problem (43): drift in the Hamiltonian.

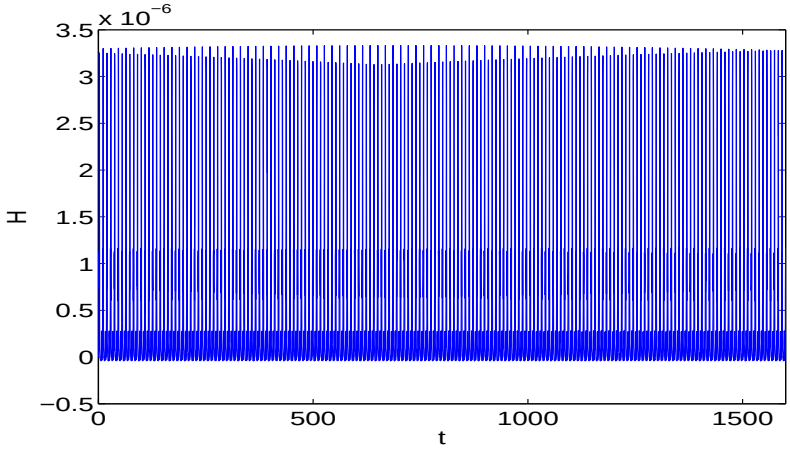

Figure 2: Fourth-order Gauss-Legendre method, $h = 0.16$, problem (43): $H \approx 10^{-6}$.

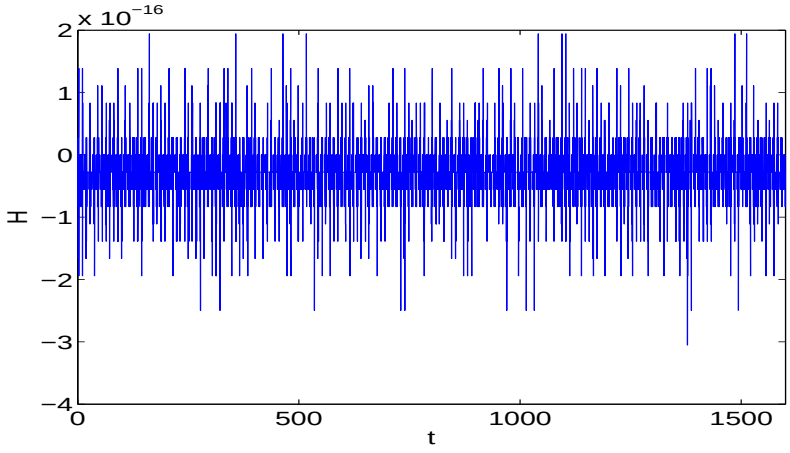

Figure 3: Fourth-order HBVM(6,2) method, $h = 0.16$, problem (43): $H \approx 10^{-16}$.

Table 1: Maximum difference between the numerical solutions obtained through the fourth-order HBVM$(k,2)$ methods based on Lobatto abscissae and Gauss-Legendre abscissae for increasing values of k, problem (45), 10^3 steps with stepsize $h = 0.1$.

k	$h = 0.1$
2	$3.97 \cdot 10^{-1}$
4	$2.29 \cdot 10^{-3}$
6	$2.01 \cdot 10^{-8}$
8	$1.37 \cdot 10^{-11}$
10	$5.88 \cdot 10^{-13}$

with $q_0 = q_{2m+1} = 0$, $m = 3$, $\omega = 50$, and starting vector

$$p_i = 0, \quad q_i = (i-1)/10, \qquad i = 1, \dots, 6.$$

In such a case, the Hamiltonian function is a polynomial of degree 4, so that the fourth-order HBVM(4,2) method, either when using the Lobatto nodes or the Gauss-Legendre nodes, is able to exactly preserve the Hamiltonian, as confirmed by the plot in Figure 6, obtained with stepsize $h = 0.05$. Conversely, by using the same stepsize, both the fourth-order Lobatto IIIA and Gauss-Legendre methods provide only an approximate conservation of the Hamiltonian, as shown in the plots in Figures 4 and 5, respectively.

5.3 Test problem 3 (non-polynomial Hamiltonian)

In the previous examples, the Hamiltonian function was a polynomial. Nevertheless, as observed above, also in this case HBVM(k,s) are expected to produce a *practical* conservation of the energy when applied to systems defined by a non-polynomial Hamiltonian function that can be locally well approximated by a polynomial. As an example, we consider the motion of a charged particle in a magnetic field with Biot-Savart potential.[24] It is defined by the Hamiltonian [2]

$$H(x,y,z,\dot{x},\dot{y},\dot{z}) = \frac{1}{2m}\left[\left(\dot{x} - \alpha\frac{x}{\varrho^2}\right)^2 + \left(\dot{y} - \alpha\frac{y}{\varrho^2}\right)^2 + \left(\dot{z} + \alpha\log(\varrho)\right)^2\right], \tag{45}$$

with $\varrho = \sqrt{x^2+y^2}$, $\alpha = e\,B_0$, m is the particle mass, e is its charge, and B_0 is the magnetic field intensity. We have used the values

$$m = 1, \qquad e = -1, \qquad B_0 = 1,$$

with starting point

$$x = 0.5, \quad y = 10, \quad z = 0, \quad \dot{x} = -0.1, \quad \dot{y} = -0.3, \quad \dot{z} = 0.$$

By using the fourth-order Lobatto IIIA method, with stepsize $h = 0.1$, a drift is again experienced in the numerical solution, as is shown in Figure 7. By using the fourth-order Gauss-Legendre method with the same stepsize, the drift disappears even though, as shown in Figure 8, the value of the Hamiltonian is preserved within an error of the order of 10^{-3}. On the other hand, when using the HBVM(6,2) method with the same stepsize, the error in the Hamiltonian decreases to an order of 10^{-15} (see Figure 9), thus giving a practical conservation. Finally, in Table 1 we list the maximum absolute difference between the numerical solutions over 10^3 integration steps, computed by the HBVM$(k,2)$ methods based on Lobatto abscissae and on Gauss-Legendre abscissae, as k grows, with stepsize $h = 0.1$. As expected, the difference tends to 0, as k increases, since the two sequences of methods tend to the same limit, given by the HBVM$(\infty,2)$ (see (24) with $s = 2$).

[24] This kind of motion causes the well known phenomenon of *aurora borealis*.

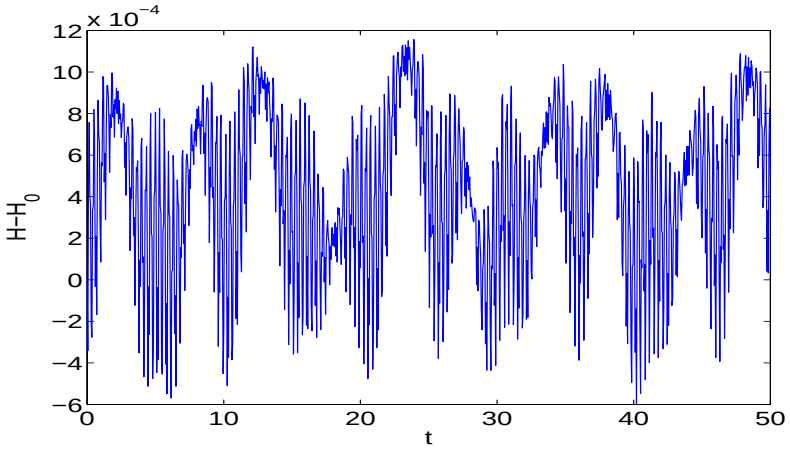

Figure 4: Fourth-order Lobatto IIIA method, $h = 0.05$, problem (44): $|H - H_0| \approx 10^{-3}$.

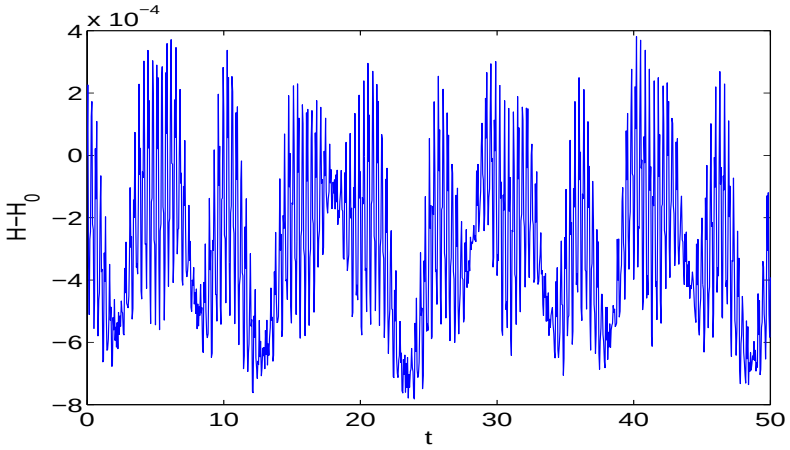

Figure 5: Fourth-order Gauss-Legendre method, $h = 0.05$, problem (44): $|H - H_0| \approx 10^{-3}$.

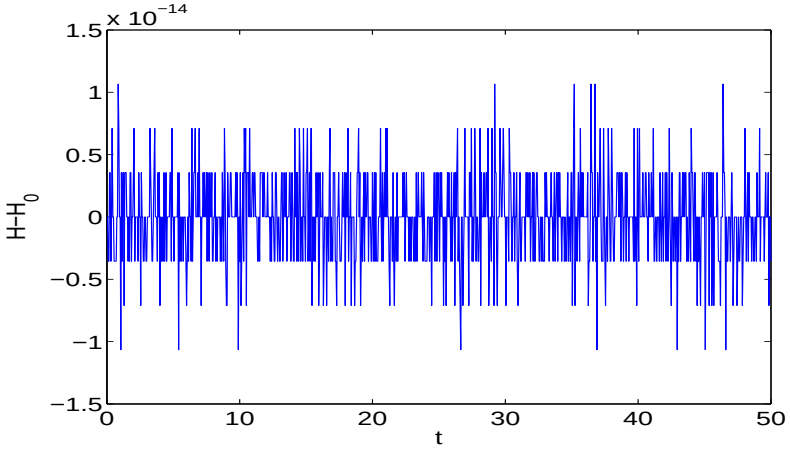

Figure 6: Fourth-order HBVM(4,2) method, $h = 0.05$, problem (44): $|H - H_0| \approx 10^{-14}$.

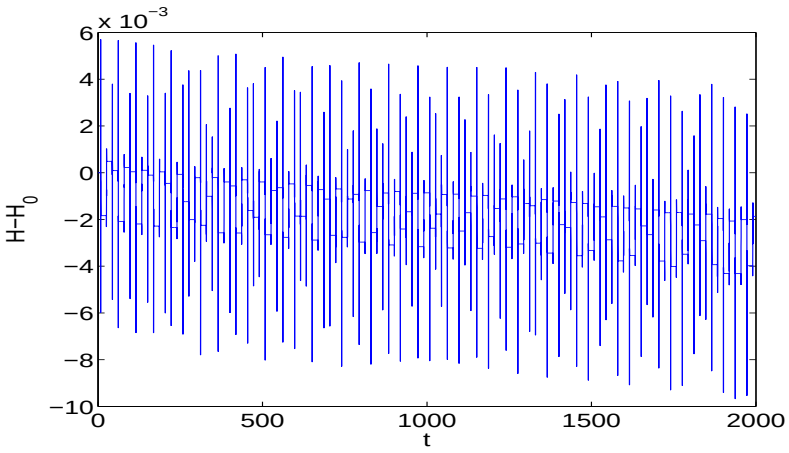

Figure 7: Fourth-order Lobatto IIIA method, $h = 0.1$, problem (45): drift in the Hamiltonian.

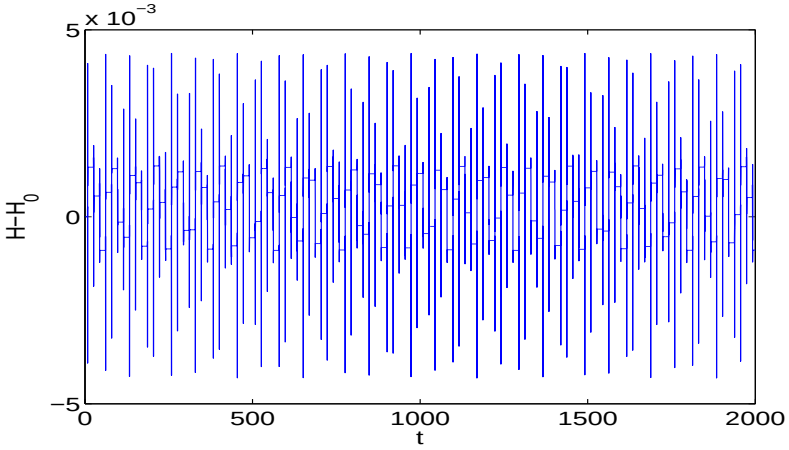

Figure 8: Fourth-order Gauss-Legendre method, $h = 0.1$, problem (45): $|H - H_0| \approx 10^{-3}$.

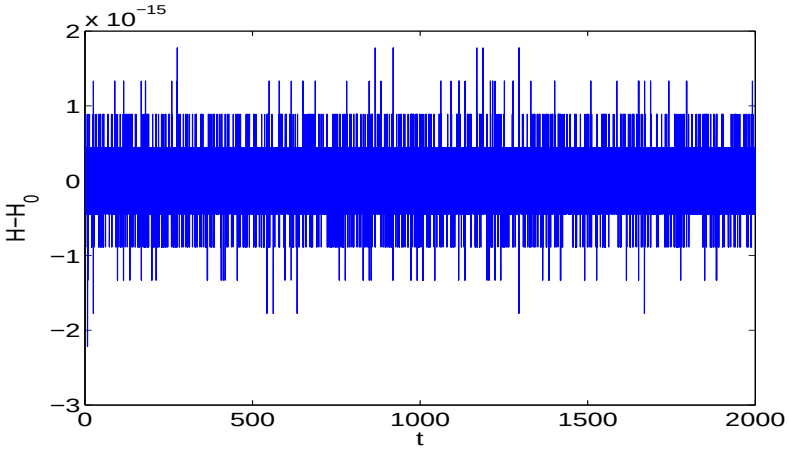

Figure 9: Fourth-order HBVM(6,2) method, $h = 0.1$, problem (45): $|H - H_0| \approx 10^{-15}$.

5.4 Test problem 4 (non-polynomial Hamiltonian)

We finally solve the Hamiltonian system (38) by using the Itho-Abe method (33), the fourth-order formula (40)–(41), and the HBVM(10,2), which has order four and degree of precision 10 (that is, according to (42), it precisely conserves the energy of polynomial Hamiltonians of degree up to 10). We have set $a = b = 1$ in formula (37), and integrated over a time interval $[0, 5000]$ with stepsize $h = 0.5$ and $(q_0, p_0) = (0.5, 0.5)$ as initial condition.

Figure 10 reports the numerical Hamiltonian function associated with the three methods. The occurrence of jumps in the first two graphs (left picture) is due to the fact that both formulae (33) and (40)–(41) may become ill-conditioned for certain values of the state vector. For example (see Figure 11), at the two consecutive times $t = 2830.5$ and $t = 2831$, the state vectors associated with the Itoh-Abe method (33) are, respectively,

$$[q_1, p_1] \simeq (0.39988668, 1.4216560)^T, \qquad [q_2, p_2] \simeq (0.39988872, 0.67130503)^T,$$

which shows that q_1 may be very close to q_2 even for large values of h. This causes some cancellation in the subtraction at the right-hand side of (33) and, hence, a jump of the subsequent branch of the numerical trajectory on a different level curve. However, since, in general, the numerical trajectory densely fills the level curve $H(y) = H(y_0)$, it may be argued that the occurrence of such jumps are systematic and frequent when the dynamics is traced over a long time. The use of finite arithmetic eventually destroys the theoretical conservation property. A similar argument may be applied to discuss the behavior of the fourth-order method (40)–(41).

Although the HBVM method does not provide a theoretical conservation of the energy, as is the case for the above cited methods, its behavior in finite arithmetic would suggest the opposite (see the right picture in Figure 10), as already emphasized at the beginning of Example 3.

6 Conclusions

In this paper, the newly introduced *Hamiltonian Boundary Value Methods (HBVMs)*, a class of numerical methods able to exactly preserve polynomial Hamiltonians of any degree, have been re-derived in a unifying framework. Such framework relies on the use of line integrals, which are approximated by suitable discrete counterparts (actually, they are exact, when the Hamiltonian is a polynomial). In this context, the limit of the methods, as the number of the so called *silent stages* tends to infinity, is easily obtained. When the underlying polynomial basis upon which the HBVM is constructed is the Lagrange basis, such limit formulae coincide with the recently introduced *Energy Preserving variant of Collocation Methods*; if instead one uses the shifted Legendre polynomial basis, the corresponding HBVMs have the highest possible order and so do their limit formulae, the *Infinity Hamiltonian Boundary Value Methods*, independently of the considered abscissae. Any limit formula, when discretized, fall into the HBVMs class. Possible extensions of the approach have been also sketched, along with a number of numerical tests. Such tests confirm that, in the limit of the silent stages tending to infinity, all HBVMs with s (unknown) *fundamental stages* tend to the *same* limit method, which is characterized by the eigenfunction (relative to the unit eigenvalue) of a certain operator, which is independent of the choice of the abscissae.

7 Acknowledgements

This work emerged from fruitful discussions with Ernst Hairer during the international conference "ICNAAM 2009", Rethymno, Crete, Greece, 18–22 September 2009. It has also benefited from his many subsequent comments. We wish also to thank an anonymous referee for the useful comments.

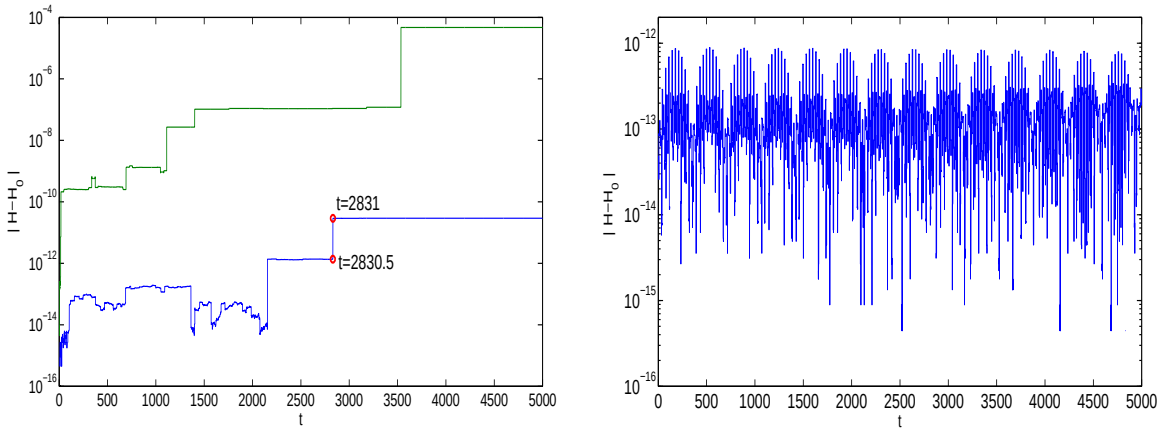

Figure 10: Left picture: absolute error of the Hamiltonian function (37) evaluated along the numerical solutions computed by the Itoh-Abe method (33) (lower curve) and formula (40)–(41) (upper curve). The jumps are symptomatic of ill-conditioning of the formulae for certain values of the solution. Right picture: the same kind of plot produced by the HBVM formula of order 4 and $k = 10$ Gaussian abscissae ($|H - H_0| \approx 10^{-12}$).

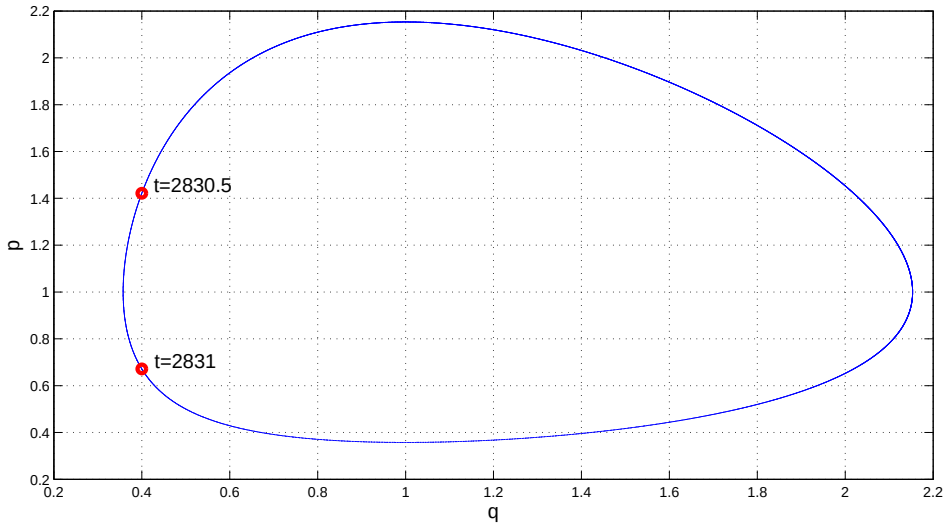

Figure 11: Trajectory in the phase plane computed by the Itoh-Abe method (33). The small circles locate the solution at the two consecutive times $t = 2830.5$ and $t = 2831$. The very close values of the variable q for such two points causes loss of significant digits in the subsequent branch of the trajectory.

References

[1] L. Brugnano, F. Iavernaro, D. Trigiante. *The Hamiltonian Boundary Value Methods (HBVMs) Homepage*. `arXiv:1002.2727`.

[2] L. Brugnano, F. Iavernaro, D. Trigiante. Analisys of Hamiltonian Boundary Value Methods (HBVMs) for the numerical solution of polynomial Hamiltonian dynamical systems. *Submitted for publication*, 2009 (`arXiv:0909.5659`).

[3] L. Brugnano, D. Trigiante. *Solving Differential Problems by Multistep Initial and Boundary Value Methods*. Gordon and Breach, Amsterdam, 1998.

[4] E. Celledoni, R.I. McLachlan, D. McLaren, B. Owren, G.R.W. Quispel, W.M. Wright. Energy preserving Runge-Kutta methods. M2AN **43** (2009) 645649.

[5] E. Faou, E. Hairer, T.-L. Pham. Energy conservation with non-symplectic methods: examples and counter-examples. *BIT Numerical Mathematics* **44** (2004) 699–709.

[6] O. Gonzales. Time integration and discrete Hamiltonian systems. *J. Nonlinear Sci.* **6** (1996) 449–467.

[7] E. Hairer. Energy-preserving variant of collocation methods. *Submitted for publication*, 2009

[8] E. Hairer, C. Lubich, G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations, 2^{nd} ed.*, Springer, Berlin, 2006.

[9] E. Hairer, G. Wanner. *Solving Ordinary Differential Equations I, 2nd ed.*, Springer, Berlin, 2000.

[10] F. Iavernaro, B. Pace. s-Stage Trapezoidal Methods for the Conservation of Hamiltonian Functions of Polynomial Type. *AIP Conf. Proc.* **936** (2007) 603–606.

[11] F. Iavernaro, D. Trigiante. High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems. *J. Numer. Anal. Ind. Appl. Math.* **4**,1-2 (2009) 87–101.

[12] T. Itoh, K. Abe. Hamiltonian-conserving discrete canonical equations based on variational difference quotients. *J. Comput. Phys.* **76** no. 1 (1988) 85–102.

[13] T. Matsuo, D. Furihata. Dissipative or conservative finite-difference schemes for complex-valued nonlinear partial differential equations. *J. Comput. Phys.* **171** no. 2 (2001) 425–447.

[14] R.I. McLachlan, G.R.W. Quispel, N. Robidoux. Geometric integration using discrete gradients. *R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci.* **357** (1999) 1021–1045.

[15] G.R.W. Quispel, D.I. McLaren. A new class of energy-preserving numerical integration methods. *J. Phys. A* **41** (2008) 04526, 7.