Journal of Computational and Applied Mathematics 236 (2012) 3905–3919

Contents lists available at SciVerse ScienceDirect

Journal of Computational and Applied Mathematics

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

Line integral methods which preserve all invariants of conservative problems☆

Luigi Brugnano [a], Felice Iavernaro [b,*]

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

[b] Dipartimento di Matematica, Università di Bari, Italy

ARTICLE INFO

Article history:
Received 15 September 2011
Received in revised form 27 February 2012

In memory of Professor Donato Trigiante

Keywords:
Ordinary differential equations
One-step methods
Hamiltonian Boundary Value Methods
Energy-preserving methods
Conservative problems
Line integral methods

ABSTRACT

Recently, the class of Hamiltonian Boundary Value Methods (HBVMs) has been introduced with the aim of preserving the energy associated with polynomial Hamiltonian systems (and, more in general, with all suitably regular Hamiltonian systems). However, many interesting problems admit other invariants besides the Hamiltonian function. It would be therefore useful to have methods able to preserve any number of independent invariants. This goal is achieved by generalizing the line-integral approach which HBVMs rely on, thus obtaining a number of generalizations which we collectively name *Line Integral Methods*. In fact, it turns out that this approach is quite general, so that it can be applied to any numerical method whose discrete solution can be suitably associated with a polynomial, such as a collocation method, as well as to any conservative problem. In particular, a completely conservative variant of both HBVMs and Gauss collocation methods is presented. Numerical experiments confirm the effectiveness of the proposed methods.

1. Introduction

Energy preserving methods have been the subject of many researches in recent years, mainly related to the numerical solution of Hamiltonian problems. The first successful attempts to derive energy preserving methods come back to "discrete gradient methods" (see [1] and references therein). More recently, energy preserving Runge–Kutta methods have been derived in [2], based on the concept of *discrete line integral*. This idea, further developed, has led to additional examples of conservative Runge–Kutta methods [3,4] and, finally, to the definition of Hamiltonian Boundary Value Methods (HBVMs) [5–12]. Limit methods of HBVMs, though using a different basis (Lagrange instead of Legendre, as is shown in [9]) are described in [13]. The latter methods can be also seen as a generalization of the "averaged vector field" described in [14,15]. A further generalization of HBVMs is described in [16].

Even though energy-conservation is an important feature for the discrete dynamical system induced by the methods, many Hamiltonian problems (and, in general, conservative problems) are characterized by the presence of multiple invariants. It would therefore be useful to devise numerical methods able to preserve all the invariants. One successful attempt in this direction has been described in [17,18] (see also [19]), where energy-preserving methods able to preserve also quadratic invariants of canonical Hamiltonian systems are defined and analyzed. A general attempt to solve the problem, based on *skew gradients* [20,21], has also been defined. It is worth mentioning that projection-type methods have also been successfully used in this case [22]. In this paper we provide a general framework for this problem, by

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

* Corresponding author.
E-mail addresses: luigi.brugnano@unifi.it (L. Brugnano), felix@dm.uniba.it (F. Iavernaro).

0377-0427/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.cam.2012.03.026

considering, as an example, the case of Hamiltonian problems with two invariants, though the procedure is straightforwardly extended to any conservative problem, and to an arbitrary number of invariants (as is shown in the numerical tests). The framework is provided by generalizing the *discrete line integral methods* resulting in HBVMs. For this reason, we name the new class of methods collectively *Line Integral Methods (LIMs)*. Among them, the straight generalization of HBVMs will be referred to as *Generalized HBVMs (GHBVMs)*. However, as will become clear, the procedure can be naturally extended to *any* discrete method, whose solution can be suitably associated with a polynomial, e.g., collocation methods. As an example, a conservative variant of Gauss collocation methods is also derived.

With this premise, the paper is organized as follows: in Section 2 the basic facts on HBVMs are recalled; then, in Section 3 LIMs are derived and analyzed, with particular attention to the conservative generalizations of HBVMs and Gauss collocation methods; finally, in Section 4 several numerical tests are reported, along with some concluding remarks.

2. Hamiltonian boundary value methods

HBVMs are here recalled by using the approach followed in [10,11], where it is shown that the methods are related to a local truncated Fourier expansion of the continuous problem. Let

$$y'(t) = f(y) \equiv J\nabla H(y(t)), \qquad y(0) = y_0 \in \mathbb{R}^{2m}, \qquad J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix} \equiv -J^T, \tag{1}$$

be a canonical Hamiltonian problem, where, for sake of simplicity, the Hamiltonian function $H(y)$ is assumed to be analytical in a region containing the solution, which is assumed to exist for all $t \geq 0$. Expand the right-hand side of (1) along an orthonormal polynomial basis $\{P_i\}$ on the interval $[0, 1]$[1]:

$$\int_0^1 P_i(x)P_j(x)\mathrm{d}x = \delta_{ij}, \qquad \deg(P_i) = i, \quad \forall i, j \geq 0, \tag{2}$$

where δ_{ij} is the Kronecker symbol. Consequently, the P_i are the shifted and scaled Legendre polynomials. One then obtains

$$y'(ch) = \sum_{j\geq 0} \gamma_j(y)P_j(c), \quad c \in [0, 1], \tag{3}$$

where the Fourier coefficients $\gamma_j(y)$ are given by

$$\gamma_j(g) = \int_0^1 P_j(\tau)f(g(\tau h))\mathrm{d}\tau, \quad j \geq 0, \tag{4}$$

after setting $g(t) = y(t)$. In (4), we use a generic vector-valued function g defined for $t \in [0, h]$, since different Fourier coefficients will be considered in the sequel.

In order to define a polynomial of given degree, say r, approximating the solution of (1), it is enough to truncate the series at the right-hand side in (3) after r terms, thus obtaining

$$\sigma'(ch) = \sum_{j=0}^{r-1} \gamma_j(\sigma)P_j(c), \quad c \in [0, 1]. \tag{5}$$

Indeed, problem (5), coupled with the initial condition $\sigma(0) = y_0$, admits a polynomial solution implicitly defined by

$$\sigma(ch) = y_0 + h\sum_{j=0}^{r-1} \gamma_j(\sigma) \int_0^c P_j(\tau)\mathrm{d}\tau, \quad c \in [0, 1],$$

with the coefficients $\{\gamma_j(\sigma)\}$ given by (4), with g replaced by σ. By considering that $P_0(c) \equiv 1$ and the orthogonality conditions (2), the new approximation y_1 at time h is then defined as

$$y_1 \equiv \sigma(h) = y_0 + h\gamma_0(\sigma).$$

By using a suitable line integral, one easily realizes that $H(y_1) = H(y_0)$. In fact, after defining (see (1))

$$\rho_j(\sigma) = \int_0^1 P_j(\tau)\nabla H(\sigma(\tau))\mathrm{d}\tau \equiv J^T\gamma_j(\sigma), \tag{6}$$

one observes that

$$H(y_1) - H(y_0) = h\int_0^1 \nabla H(\sigma(ch))^T\sigma'(ch)\mathrm{d}c = h\sum_{j=0}^{r-1} \rho_j(\sigma)^T\gamma_j(\sigma) = h\sum_{j=0}^{r-1} \gamma_j(\sigma)^T J\gamma_j(\sigma) = 0, \tag{7}$$

where the last three equalities follow, respectively, from (5), (6), and considering that matrix J is skew-symmetric. Furthermore, the following result can be proved (see, e.g., [11]).

Theorem 1. $y(h) - \sigma(h) = O(h^{2r+1})$.

[1] More general orthonormal bases can be also considered.

2.1. Discretization

Let us rewrite formula (5) by making the expression of $\gamma_j(\sigma)$ in (4) explicit:

$$\sigma'(ch) = \sum_{j=0}^{r-1} P_j(c) \int_0^1 P_j(\tau) f(\sigma(\tau h)) \mathrm{d}\tau, \quad c \in [0, 1].$$

This clearly reveals that this formula does not yet provide a practical numerical method, unless the integrals are approximated by means of a suitable quadrature formula. By using a quadrature formula defined at the abscissae $\{c_1, \ldots, c_k\}$, and having order of accuracy q (that is, exact for polynomials of degree $q-1$), one then obtains (see (4))

$$\gamma_j(\sigma) - \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f(\sigma_\ell) \equiv \gamma_j(\sigma) - \hat{\gamma}_j \equiv \Delta_j(h) = O(h^{q-j}), \quad j = 0, \ldots, r-1, \tag{8}$$

where the $\{b_\ell\}$ are the quadrature weights. We will write, hereafter,

$$\sigma_\ell \equiv \sigma(c_\ell), \quad \ell = 1, \ldots, k. \tag{9}$$

Clearly, if we place the weights at the Gauss nodes in $[0, 1]$, which we shall assume in the sequel, then $q = 2k$, and the quadrature is exact for all polynomial Hamiltonians of degree

$$\nu \le \frac{2k}{r}. \tag{10}$$

In such a case, if we denote

$$u'(ch) = \sum_{j=0}^{r-1} P_j(c) \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f(u_\ell), \tag{11}$$

with an obvious meaning of u_ℓ (see (9)), one obtains that $\sigma \equiv u$. Otherwise, the two polynomials will differ. However, by choosing k large enough, one can approximate the integrals to within machine precision, thus obtaining a *practical* conservation of all suitably regular Hamiltonian functions (see Theorem 3). This leads to only a slight increase in the complexity of the nonlinear system to be solved, which can be seen to have (block) size r, independently of k [5,8,12,23].

Eq. (11) defines a HBVM(k, r) method at the k Gauss-nodes. With such a choice of the nodes, HBVM(r, r) turns out to be the Gauss methods of order $2r$ [9].[2] When $k > r$, the resulting method may still be cast as a Runge–Kutta method, if preferred (see for example [12,23]). Concerning the order of accuracy, the following results hold true (see, e.g., [11]).

Theorem 2. $y(h) - u(h) = O(h^{2r+1})$, $\forall k \ge r$.

Theorem 3. *For all polynomial Hamiltonians satisfying (10), one obtains $H(u(h)) = H(y_0)$. Conversely, for all suitably regular Hamiltonian functions, $H(u(h)) - H(y_0) = O(h^{2k+1})$, $\forall k \ge r$.*

3. Line integral methods

We now generalize the previous formulae and methods, in order to obtain new ones able to preserve, in the discrete solution, more than one (smooth) invariant of the continuous dynamical system. We shall discuss the case of two invariants (e.g., the Hamiltonian $H(y)$ and a second invariant $L(y)$), though the argument can be straightforwardly extended to any number of invariants and, evidently, to any suitable function $f(y)$ in (1).

The key idea is again to exploit the properties of the line integral (and its discrete counterpart), originally used to derive HBVMs. In more detail, the dynamical system induced by (1) admits a (smooth) invariant $L(y)$ if and only if, along any trajectory $y(t)$,

$$\frac{\mathrm{d}}{\mathrm{d}t} L(y(t)) = \nabla L(y(t))^T f(y(t)) = 0, \quad \forall t \ge 0. \tag{12}$$

For our purposes, since we shall consider discrete-time dynamical systems, this result can be more conveniently stated in terms of a corresponding line integral:

$$L(y(h)) - L(y_0) = h \int_0^1 \nabla L(y(\tau h))^T y'(\tau h) \mathrm{d}\tau = \sum_{j \ge 0} \phi_j(y)^T \gamma_j(y) = 0, \tag{13}$$

where we have used (3), (4), and the following expansion:

$$\nabla L(y(ch)) = \sum_{j \ge 0} P_j(c) \int_0^1 P_j(\tau) \nabla L(y(\tau h)) \mathrm{d}\tau \equiv \sum_{j \ge 0} P_j(c) \phi_j(y), \quad c \in [0, 1]. \tag{14}$$

[2] HBVMs defined at Lobatto nodes were previously considered in [5].

We also need the following result concerning the Fourier coefficients (4), (6) and (14).

Lemma 1. *Under suitable regularity assumptions for a given function $G(t)$, one has*

$$\int_0^1 G(\tau h)P_j(\tau)\mathrm{d}\tau = O(h^j), \quad j \geq 0.$$

Consequently, from (3) – (4) and (14) one obtains:

$$\sum_{j=0}^{r-1} \phi_j(\cdot)^T \gamma_j(\cdot) = O(h^{2r}). \tag{15}$$

Proof. The (very simple) proof of the first part can be found in [10,11]. The second equation then easily follows from (13). □

We now derive particular instances of Line Integral Methods: the straight generalization of HBVMs, and that of Gauss collocation methods.

3.1. Generalized HBVMs (GHBVMs)

We have seen that HBVMs can be obtained from formula (5), whose solution satisfies $H(\sigma(h)) = H(y_0)$ (at least, in the case of Hamiltonian problems) but not, in general $L(\sigma(h)) = L(y_0)$. The basic idea is now that of perturbing one of the coefficients in the expansion (5), in order to obtain *both*

$$H(\sigma(h)) = H(y_0) \quad \text{and} \quad L(\sigma(h)) = L(y_0). \tag{16}$$

The perturbation will be done by using a linear combination of the corresponding coefficients of the expansions of $\nabla H(\cdot)$ and $\nabla L(\cdot)$. Let us then assume, for sake of simplicity, to perturb the first coefficient of the expansion in (5),[3] so that we obtain the new expansion (we continue to denote by σ the new resulting polynomial)

$$\sigma'(ch) = \sum_{j=0}^{r-1} P_j(c)\gamma_j(\sigma) + P_0(c)\left(x_1\rho_0(\sigma) + x_2\phi_0(\sigma)\right), \quad c \in [0,1], \tag{17}$$

in place of (5). Actually, also the scalar coefficients x_1 and x_2 in (17) do depend on σ: they will be determined in order to obtain the conservation conditions (16) which, using (7) and (13), read

$$\int_0^1 \nabla H(\sigma(ch))^T \sigma'(ch)\mathrm{d}c = 0 \quad \text{and} \quad \int_0^1 \nabla L(\sigma(ch))^T \sigma'(ch)\mathrm{d}c = 0. \tag{18}$$

Substituting (17) into (18), and defining the matrix[4]

$$A \equiv (\rho_0,\ \phi_0), \tag{19}$$

yields the following set of equations:

$$A^T A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = -\begin{pmatrix} \sum_{j=0}^{r-1} \rho_j(\sigma)^T \gamma_j(\sigma) \\ \sum_{j=0}^{r-1} \phi_j(\sigma)^T \gamma_j(\sigma) \end{pmatrix} \equiv \begin{pmatrix} 0 \\ O(h^{2r}) \end{pmatrix}, \tag{20}$$

where the rightmost hand side comes from (7) and Lemma 1.[5] Notice that the two *scalar* equations in (20) are actually nonlinear due to the presence of $\phi_j(\sigma)$ and $\gamma_j(\sigma)$ at the right-hand side, and $\phi_0(\sigma)$, $\rho_0(\sigma)$ defining A. They must be coupled with the (block) nonlinear equations

$$\begin{aligned} \gamma_j(\sigma) &= \int_0^1 P_j(\tau) f(\sigma(\tau h))\mathrm{d}\tau, \qquad \rho_j(\sigma) = \int_0^1 P_j(\tau)\nabla H(\sigma(\tau h))\mathrm{d}\tau, \\ \phi_j(\sigma) &= \int_0^1 P_j(\tau)\nabla L(\sigma(\tau h))\mathrm{d}\tau, \quad j = 0,\ldots,r-1, \end{aligned} \tag{21}$$

to form a nonlinear system that must be solved at each step of the integration procedure.[6] For this purpose, we shall made the following simplifying assumption, which essentially states that the two manifolds

[3] This choice, indeed, is the most recommendable, as is shown in the sequel.

[4] In the case of ℓ invariants, A would have ℓ columns, given by the Fourier coefficients of the corresponding gradients.

[5] For general (non Hamiltonian) problems, the first entry of the vector at the right-hand side in (20) would be also $O(h^{2r})$.

[6] Actually, this dimension could be reduced, as it will be shown elsewhere, where the efficient implementation of the methods will be studied.

$$H(y) = H(y_0) \quad \text{and} \quad L(y) = L(y_0), \tag{22}$$

are not tangent along the path $\sigma(ch)$, $c \in [0, 1]$.

Assumption 1. Matrix A defined in (19) has full rank, so that A^TA is symmetric and positive definite.

The arguments can be suitably modified to cope with the general case. We skip them here, for sake of brevity, even though the basic idea essentially consists in considering the pseudo-inverse of matrix A^TA, in place of its inverse. From Assumption 1 one then obtains

$$x_1 = O(h^{2r}), \qquad x_2 = O(h^{2r}), \tag{23}$$

so that in (17) the perturbation of the $O(h^0)$ coefficient $\gamma_0(\sigma)$ is $O(h^{2r})$ and, therefore, very small, as $h \to 0$.

Remark 1. We observe that in general, if the matrix $A_j = \left(\rho_j, \phi_j\right)$ has full rank, $A_j^TA_j$ is symmetric and positive definite, with $O(h^{2j})$ entries. Then its inverse has $O(h^{-2j})$ entries and consequently, perturbing the coefficient $\gamma_j(\sigma)$ instead of $\gamma_0(\sigma)$, would result in a $O(h^{2(r-j)})$ perturbation of this $O(h^j)$ coefficient. One then concludes that the choice $j = 0$ is that providing the smallest perturbation, both absolute and relative, as $h \to 0$.

Remark 2. A further interesting remark concerns the geometrical interpretation of (17). By taking into account that (see (21))

$$\rho_0(\sigma) = \int_0^1 \nabla H(\sigma(\tau h))\mathrm{d}\tau, \qquad \phi_0(\sigma) = \int_0^1 \nabla L(\sigma(\tau h))\mathrm{d}\tau,$$

the (integral) mean value theorem and the fact that $\sigma(\tau h) = y(\tau h) + O(h^{2r+1})$ suggest that the vectors ρ_0 and ϕ_0 are, in mean, orthogonal to the manifolds (22) in a neighborhood of diameter h close to y_0. Thus the perturbation term $x_1\rho_0 + x_2\phi_0$ somehow forces $\sigma'(ch)$ to have a non-null component along a direction that points straight towards the manifolds (22). System (20) tunes the values of the parameters x_1 and x_2 in order to get the conservation conditions (16).

The next theorem states that the perturbation introduced in σ' to get the conservation of L does not alter the order of the resulting method. The proof strictly follows that of Theorem 1 in [11].

In the sequel, $y(t, s, z)$ will denote the solution at time t of the problem $y' = f(y)$ with initial condition $y(s) = z$, while $\Phi(t, s, z)$ will denote the fundamental matrix function of the associated variational problem, with initial condition $\Phi(s, s, z) = I$, that is $\Phi(t, s, z) = \frac{\partial}{\partial z}y(t, s, z)$.

Theorem 4. *Under Assumption 1,* $y(h) - \sigma(h) = O(h^{2r+1})$.

Proof. We have[7]

$$\begin{aligned}
y(h) - \sigma(h) &= y(h, 0, y_0) - y(h, h, \sigma(h)) = -\int_0^h \frac{\mathrm{d}}{\mathrm{d}t}y(h, t, \sigma(t))\mathrm{d}t \\
&= -\int_0^h \left[\frac{\partial}{\partial s}y(h, t, \sigma(t)) + \frac{\partial}{\partial z}y(h, t, \sigma(t))\,\sigma'(t)\right]\mathrm{d}t \\
&= -h\int_0^1 \left[\frac{\partial}{\partial s}y(h, \tau h, \sigma(\tau h)) + \frac{\partial}{\partial z}y(h, \tau h, \sigma(\tau h))\,\sigma'(\tau h)\right]\mathrm{d}\tau \\
&= h\int_0^1 \Phi(h, \tau h, \sigma(\tau h))\left[f(\sigma(\tau h)) - \sigma'(\tau h)\right]\mathrm{d}\tau \\
&= h\int_0^1 \Phi(h, \tau h, \sigma(\tau h))\left[\sum_{j\ge r} P_j(\tau)\gamma_j(\sigma) - x_1\rho_0(\sigma) - x_2\phi_0(\sigma)\right]\mathrm{d}\tau \\
&= h\sum_{j\ge r}\left[\int_0^1 \Phi(h, \tau h, \sigma(\tau h))P_j(\tau)\mathrm{d}\tau\right]\gamma_j(\sigma) + O(h^{2r+1}) = O(h^{2r+1}),
\end{aligned}$$

by virtue of (3), (5), Lemma 1, and (23). □

[7] Hereafter and in the sequel, the notation such as $\frac{\partial}{\partial s}y(h, t, \sigma(t))$ will denote the partial derivative of $y(t, s, z)$ with respect to s, evaluated at $t = h$, $s = t$ and $z = \sigma(t)$ and analogously for the partial derivative of $y(t, s, z)$ with respect to z.

3.2. Discretization

In order to obtain actual numerical methods, we need to approximate the integrals appearing in (21). Again, let us assume to approximate them by means of a Gauss quadrature formula with $k \geq r$ nodes $\{c_\ell\}$ and weights $\{b_\ell\}$, thus obtaining (see (9))

$$\begin{aligned}
&\rho_j(\sigma) - \sum_{\ell=1}^{k} b_\ell P_j(c_\ell)\nabla H(\sigma_\ell) \equiv \rho_j(\sigma) - \hat{\rho}_j = O(h^{2k-j}), \\
&\phi_j(\sigma) - \sum_{\ell=1}^{k} b_\ell P_j(c_\ell)\nabla L(\sigma_\ell) \equiv \phi_j(\sigma) - \hat{\phi}_j = O(h^{2k-j}), \quad j = 0, \dots, r-1,
\end{aligned} \tag{24}$$

besides (8) (with $q = 2k$). Consequently, the numerical method defines the polynomial $u(ch)$ of degree r, satisfying

$$u'(ch) = \sum_{j=0}^{r-1} P_j(ch)\hat{\gamma}_j + \hat{x}_1\hat{\rho}_0 + \hat{x}_2\hat{\phi}_0, \quad c \in [0, 1], \tag{25}$$

in place of (17). By using a similar argument as the one exploited to derive (23), one proves that $\hat{x}_i = x_i + O(h^{2k}) = O(h^{2r})$, $i = 1, 2$. Consequently, from (25) and (8) (with $q = 2k$), one obtains, for all $k \geq r$,

$$\begin{aligned}
u'(ch) &= \sum_{j=0}^{r-1} P_j(ch)\gamma_j(u) - \sum_{j=0}^{r-1} P_j(ch)\Delta_j(h) + x_1\rho_0(u) + x_2\phi_0(u) + O(h^{2k}), \\
&= \sum_{j=0}^{r-1} P_j(ch)\gamma_j(u) - \sum_{j=0}^{r-1} P_j(ch)\Delta_j(h) + O(h^{2r}), \quad c \in [0, 1].
\end{aligned} \tag{26}$$

The following result can be proved, by considering that Assumption 1 holds true also for the discrete approximations, for h suitably small and/or k large enough (compare with Theorem 2 for HBVMs).

Theorem 5. *Under Assumption 1, $y(h) - u(h) = O(h^{2r+1})$, for all $k \geq r$.*

Proof. We adopt the same notation used in Theorem 4. From (26) one has, for all $k \geq r$:

$$\begin{aligned}
y(h) - u(h) &= y(h, 0, y_0) - y(h, h, u(h)) = -\int_0^h \frac{\mathrm{d}}{\mathrm{d}t} y(h, t, u(t))\mathrm{d}t \\
&= -\int_0^h \left[\frac{\partial}{\partial s} y(h, t, u(t)) + \frac{\partial}{\partial z} y(h, t, u(t))\, u'(t)\right]\mathrm{d}t \\
&= -h\int_0^1 \left[\frac{\partial}{\partial s} y(h, \tau h, u(\tau h)) + \frac{\partial}{\partial z} y(h, \tau h, u(\tau h))\, u'(\tau h)\right]\mathrm{d}\tau \\
&= h\int_0^1 \Phi(h, \tau h, u(\tau h))\left[f(u(\tau h)) - \sum_{j=0}^{r-1} P_j(\tau)\gamma_j(u) + \sum_{j=0}^{r-1} P_j(\tau)\Delta_j(h) + O(h^{2r})\right]\mathrm{d}\tau \\
&= h\int_0^1 \Phi(h, \tau h, \sigma(\tau h))\left[\sum_{j\geq r} P_j(\tau)\gamma_j(u) + \sum_{j=0}^{r-1} P_j(\tau)\Delta_j(h) + O(h^{2r})\right]\mathrm{d}\tau \\
&= h\sum_{j\geq r}\left[\int_0^1 \Phi(h, \tau h, \sigma(\tau h))P_j(\tau)\mathrm{d}\tau\right]\gamma_j(u) + h\sum_{j=0}^{r-1}\left[\int_0^1 \Phi(h, \tau h, \sigma(\tau h))P_j(\tau)\mathrm{d}\tau\right]\Delta_j(h) + O(h^{2r+1}) \\
&= O(h^{2k+1}) + O(h^{2r+1}) = O(h^{2r+1}),
\end{aligned}$$

by virtue of Lemma 1, and (8) with $q = 2k$. □

Concerning the invariants, one has (compare to Theorem 3 for HBVMs):

Theorem 6. *Under Assumption 1, if both H and L are polynomial invariants whose degree, say ν, satisfies (10), then $H(u(h)) = H(y_0)$ and $L(u(h)) = L(y_0)$; differently, $H(u(h)) - H(y_0) = O(h^{2k+1}) = L(u(h)) - L(y_0)$, for all $k \geq r$, provided that both H and L are suitably regular.*

Proof. The first part of the proof follows by considering that, in such hypotheses, all the integrals appearing in (21) are exactly computed, so that $u \equiv \sigma$ (see (17)). Concerning the second part, we only prove the first equality, since the same arguments apply to every invariant. From (26), one has, for all $k \geq r$:

$$\begin{aligned} H(u(h)) - H(y_0) &= h\int_0^1 \nabla H(u(\tau h))^T u'(\tau h)\mathrm{d}\tau \\ &= h\int_0^1 \nabla H(u(\tau h))^T \left[\sum_{j=0}^{r-1} P_j(\tau)\left(\gamma_j(u) - \Delta_j(h)\right) + x_1\rho_0(u) + x_2\phi_0(u) + O(h^{2k})\right]\mathrm{d}\tau \\ &= h\overbrace{\left[\sum_{i=0}^{r-1}\rho_j(u)^T\gamma_j(u) + x_1\rho_0(u)^T\rho_0(u) + x_2\rho_0(u)^T\phi_0(u)\right]}^{=0,(\text{see (20)})} - h\sum_{j=0}^{r-1}\rho_j(u)^T\Delta_j(h) + O(h^{2k+1}) \\ &= h\sum_{j=0}^{r-1} O(h^j)\,O(h^{2k-j}) + O(h^{2k+1}) = O(h^{2k+1}). \quad \square \end{aligned}$$

3.3. Generalized collocation methods

The above arguments and results can be easily adapted to derive a conservative extension of classical collocation methods, which we sketch below. Again, without loss of generality, we shall consider Hamiltonian problems with two (smooth) invariants (the Hamiltonian and another one, i.e., (16)). Finally, to make the arguments as simple as possible, we shall confine ourselves to Gauss methods, though in principle, any collocation method could be considered, with minor modifications. To begin with, let us consider the Gauss method collocating at the r Gauss abscissae $\{\hat{c}_i\}$ in $[0, 1]$. As was outlined at the end of Section 2, the collocating polynomial σ of degree r associated with this method satisfies (compare to (4)–(5))

$$\sigma'(ch) = \sum_{j=0}^{r-1} P_j(c)\hat{\gamma}_j(\sigma), \quad c \in [0, 1], \tag{27}$$

with

$$\hat{\gamma}_j(\sigma) = \sum_{i=1}^{r} \hat{b}_i P(\hat{c}_i) f(\hat{\sigma}_i), \quad j = 0, \ldots, r-1,$$

where $\hat{\sigma}_i = \sigma(\hat{c}_i)$, $i = 1, \ldots, r$, and the $\{\hat{b}_i\}$ are the corresponding Gauss quadrature weights. It is well-known that such methods are not conservative, unless the Hamiltonian is quadratic. Nevertheless, (15) in Lemma 1 continues to hold with γ_j replaced by $\hat{\gamma}_j$, so that, by using again the line integral approach, we can introduce a suitable correction that makes the resulting method able to conserve any number of invariants. In the present context we again impose the line-integral conditions (18), in order to obtain the conservation properties (16). Repeating the steps presented in Section 3.1, we modify (27) as follows:

$$\sigma'(ch) = \sum_{j=0}^{r-1} P_j(c)\hat{\gamma}_j(\sigma) + P_0(c)\left(x_1\rho_0(\sigma) + x_2\phi_0(\sigma)\right), \quad c \in [0, 1]. \tag{28}$$

The coefficients x_1 and x_2 that provide (18) are the solution of the following set of two *scalar* nonlinear equations (compare to (20)):

$$A^T A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = -\begin{pmatrix} \sum_{j=0}^{r-1} \rho_j(\sigma)^T\hat{\gamma}_j(\sigma) \\ \sum_{j=0}^{r-1} \phi_j(\sigma)^T\hat{\gamma}_j(\sigma) \end{pmatrix} \equiv O(h^{2r}), \tag{29}$$

with matrix A still defined by (19). Under Assumption 1, A^TA is symmetric and positive definite and thus the statement presented in Theorem 4 holds in the present case too, as is easily shown by slightly modifying its proof.

Remark 3. For sake of completeness, we mention that if we compute the polynomial (28) at the Gauss abscissae $\{\hat{c}_i\}$, then we obtain the more "familiar" form of the method

$$\sigma'(\hat{c}_i h) = f(\sigma(\hat{c}_i h)) + x_1\rho_0(\sigma) + x_2\phi_0(\sigma), \quad i = 1, \ldots, r, \tag{30}$$

where we have also taken into account that $P_0(c) \equiv 1$. This form further emphasizes the connection between the new conserving formulae and the original collocation ones and also suggests an interpretation and a possible implementation of the new formulae. In fact, suppose to initially set $x_1^{(0)} = x_2^{(0)} = 0$: then (30) becomes the standard Gauss method in the unknown σ and whose solution we denote σ_1. Correspondingly, we denote by $x_1^{(1)}$ and $x_2^{(1)}$ the solution of the linear system (29) where both A and the right hand side have been evaluated at $\sigma = \sigma_1$. We can now iterate the process and consider the sequence of systems

$$\sigma'_{k+1}(\hat{c}_i h) = f(\sigma_{k+1}(\hat{c}_i h)) + x_1^{(k)}\rho_0(\sigma_k) + x_2^{(k)}\phi_0(\sigma_k), \quad i = 1, \ldots, r,\ k = 1, 2, \ldots. \tag{31}$$

Thus each formula in the sequence amounts to the application of the Gauss method to the modified (perturbed) problem $y' = F_k(y)$, where $F_k(y) = f(y) + x_1^{(k)}\rho_0(\sigma_k) + x_2^{(k)}\phi_0(\sigma_k)$. Since $\sigma = \lim_{k\to\infty}\sigma_k$ is $O(h^{2r})$-close to σ_1, the polynomial σ_k can be assumed as a very accurate initial guess while solving the nonlinear system associated with (31) and the convergence will be attained without drastically increasing the overall cost per step related to the implementation of the Gauss method.[8]

The discretization issue strictly follows similar steps as those seen in Section 3.2: one considers a set of $k \geq r$ abscissae $\{c_\ell\}$, say at the k Gauss points in [0, 1], thus approximating the integrals as in (24). One then obtains a numerical method, which is formally still given by (25), approximating (28). It turns out that the resulting method still has order $2r$ and is able to preserve polynomial invariants of degree ν satisfying (10). In the non-polynomial case, Theorem 6 continues formally to hold, so that a *practical* conservation of any suitably smooth invariant may be obtained, provided that k is large enough.[9]

We shall refer to such methods as CGAUSS(r, k) (i.e., *conservative variant of the Gauss method with r stages and quadrature with k nodes*).

4. Numerical tests

We here report some numerical tests, to show the behavior of the methods on different problems having a number of invariants of motion. We emphasize that the conservation of each invariant requires that a scalar equation, such as the one at (21) for the function $L(y)$, must be considered during the formulation of the method. The next example shows different possibilities, in terms of conservation properties, since the dynamical system possesses more than two independent first integrals.

4.1. Example 1

As first example, we consider the well-known Kepler problem, with Hamiltonian

$$H(y) \equiv H(q_1, q_2, p_1, p_2) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \tag{32}$$

which admits, besides the Hamiltonian function, another constant of motion given by the angular momentum,

$$L(y) \equiv L(q_1, q_2, p_1, p_2) = q_1 p_2 - q_2 p_1. \tag{33}$$

The values of such constants of motion depend on the initial condition. In particular, starting at

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

one obtains a periodic solution of period 2π, given by an ellipse with eccentricity e in the (q_1, q_2)-plane (see, for example, [24]). We first use the value $e = 0.6$ and compare the following fourth-order methods with constant stepsize $h = \pi/50$:

- the symplectic 2-stage Gauss method, GAUSS4 (i.e., HBVM(2, 2)), which is not energy-preserving but preserves quadratic invariants and, therefore, the angular momentum $L(y)$;
- the HBVM(8, 2) method, which is *practically* energy-preserving, for the used stepsize. However, it does not preserve the angular momentum $L(y)$;
- the GHBVM(8, 2) method, which is practically *both* energy and angular momentum-preserving, for the given stepsize;
- the conservative variant of Gauss method with two stages and 8 quadrature nodes, CGAUSS(2, 8), which is practically *both* energy and angular momentum-preserving, for the given stepsize.

[8] Actually, in performing the numerical tests, we have considered a similar though not identical procedure.

[9] As before, here *practical* conservation means that the errors due to the discretization are comparable to round-off errors. Namely, in finite precision arithmetic the given function is undistinguishable from the polynomial approximation induced by the method.

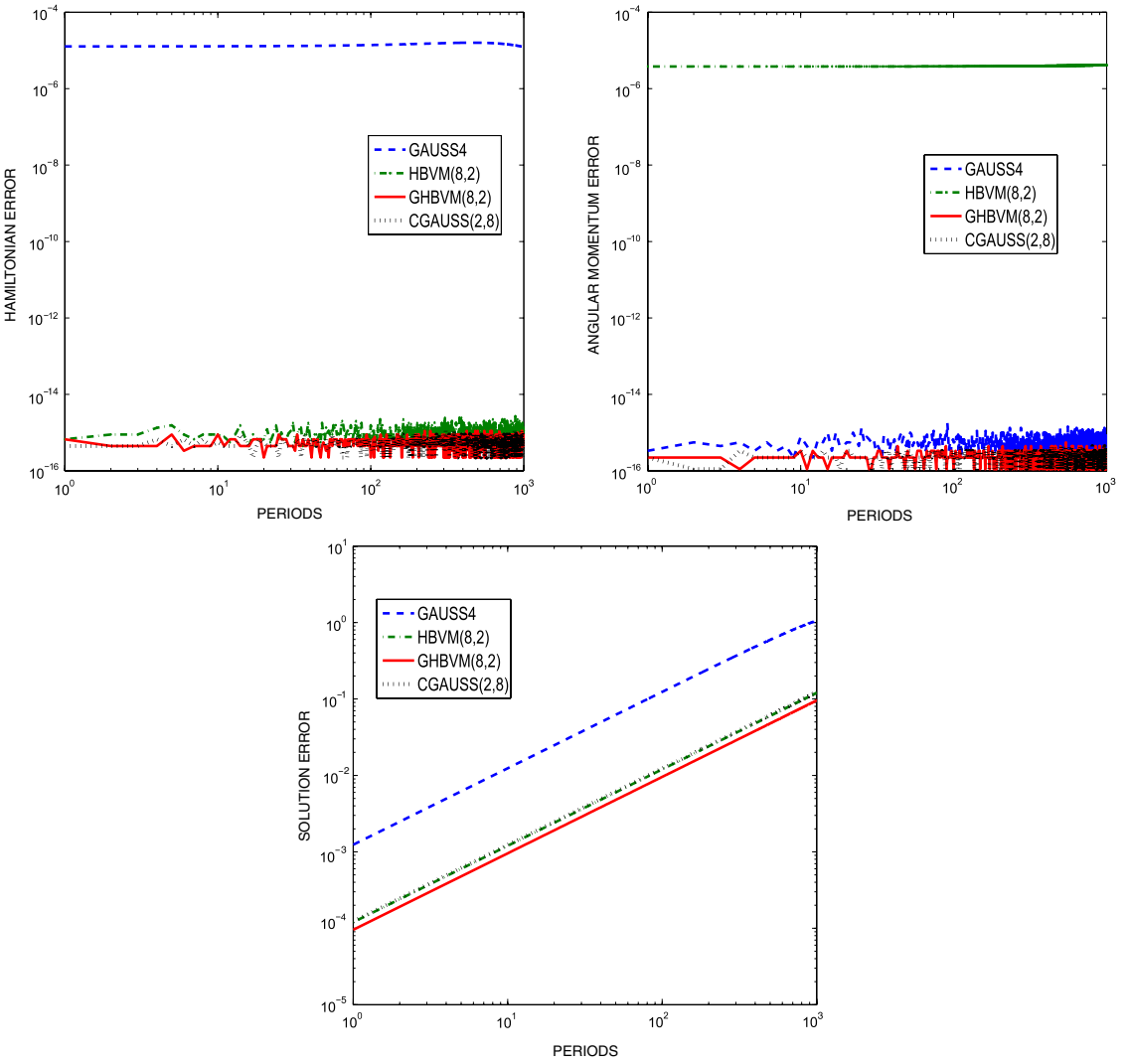

Fig. 1. Errors in the Hamiltonian (first plot), angular momentum (second plot), and solution (third plot), over a 10^3 periods integration of the Kepler problem ($e = 0.6$), by using the following fourth order methods: GAUSS4, HBVM(8, 2), GHBVM(8, 2), and CGAUSS(2, 8), with a constant stepsize $h = \pi/50$.

We integrate the problem over 10^3 periods, solving the nonlinear systems associated with the methods by fixed-point iteration. All methods converge approximately in the same number of iterations (GAUSS4 and CGAUSS(2, 8): 9.5 iterations per step; HBVM(8, 2) and GHBVM(8, 2) less then 9.7 iterations per step). The three plots in Fig. 1 summarize the measured errors in the computed solution:

- the first plot shows the Hamiltonian error, thus confirming that HBVM(8, 2), GHBVM(8, 2), and CGAUSS(2, 8) are practically energy-conserving, whereas GAUSS4 is not (though the energy error is bounded);
- the second plot regards the angular momentum error and confirms that GAUSS4, CGAUSS(2, 8), and GHBVM(8, 2) conserve this invariant, whereas HBVM(8, 2) does not (though the error in the angular momentum is bounded);
- in the third plot is the error in the computed solution. All the energy-preserving methods are much more accurate than the (symplectic) GAUSS4 method. Moreover, the GHBVM(8, 2) method is slightly more accurate than HBVM(8, 2) and CGAUSS(2, 8) (whose errors are comparable).

A constant stepsize implementation, however, turns out to be inefficient when the eccentricity e is close to 1. In such a case, a variable stepsize implementation would be more appropriate. A standard way of selecting the stepsize is given, for example, by the formula

$$h_{\text{new}} = 0.85 \cdot h_{\text{cur}} \left(\frac{\text{tol}}{\text{err}} \right)^{\frac{1}{p+1}}, \tag{34}$$

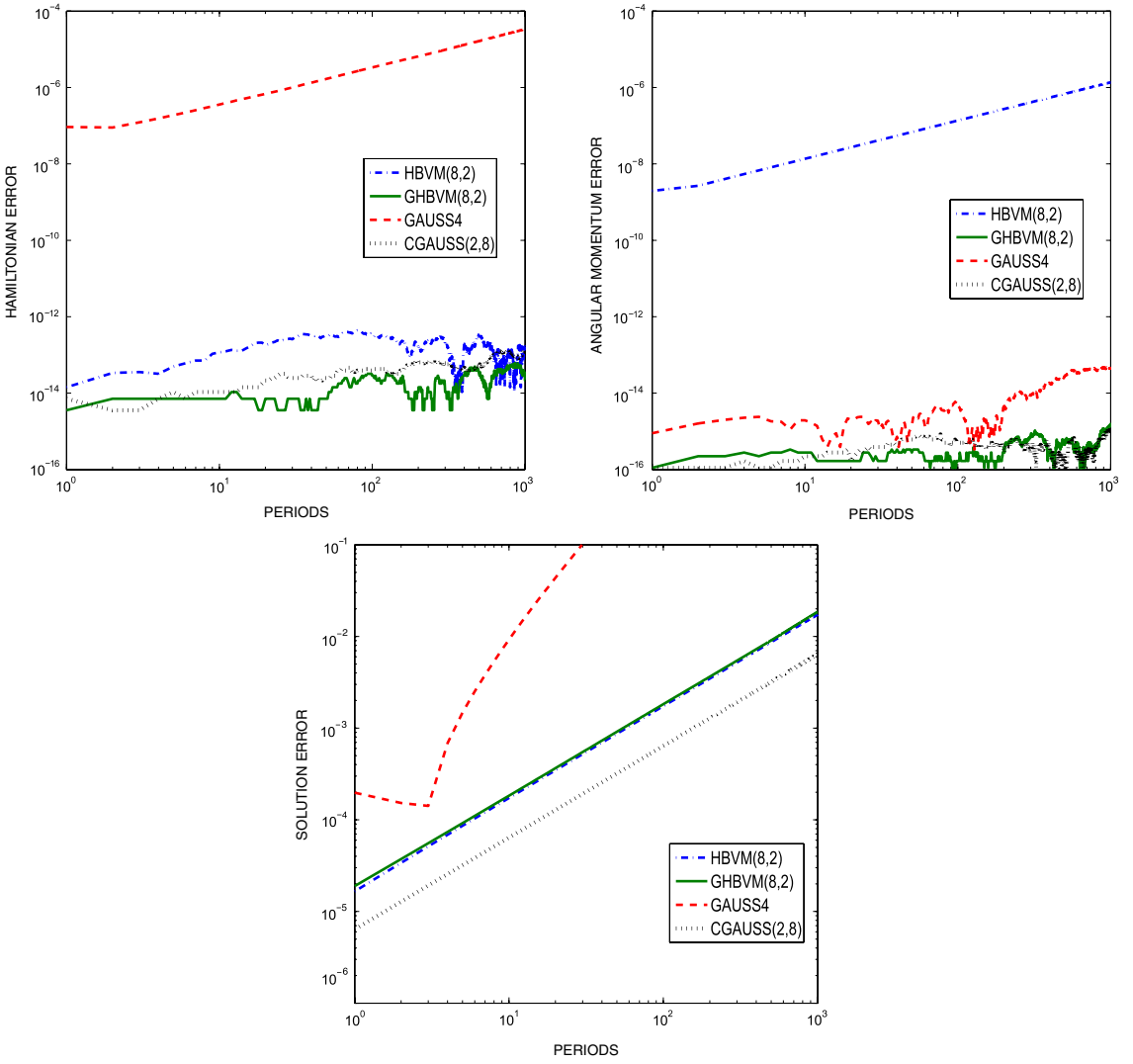

Fig. 2. Errors in the Hamiltonian (first plot), angular momentum (second plot), and solution (third plot), over a 10^3 periods integration of the Kepler problem ($e = 0.95$), by using the fourth-order HBVM(8, 2), GHBVM(8, 2), and CGAUSS(2, 8) methods, with the standard variable stepsize selection (34).

where h_{cur} is the current stepsize, h_{new} is the new stepsize, tol is the prescribed tolerance for the local error, whose estimate (described below) is given by err, p is the order of the method and, finally, 0.85 is a safety factor. Such a choice is not recommended for symplectic methods (such as GAUSS4), since it induces a drift in the Hamiltonian function and a quadratic error growth in the solution (see, e.g., [24, pp. 303–305]). Conversely, numerical tests with energy-preserving methods seem to show a more favorable situation [10,11,19]. We here compare the variable stepsize implementation, performed by (34), of the fourth-order ($p = 4$) HBVM(8, 2), GHBVM(8, 2), and CGAUSS(2, 8) methods for numerically approximating the Kepler problem with eccentricity $e = 0.95$ over 10^3 periods. For the sake of completeness, we also report the results obtained by using the GAUSS4 method. We choose $h_0 = 10^{-4}$ as initial stepsize and tolerance tol $= 10^{-10}$ for HBVM(8, 2), GHBVM(8, 2), whereas tol $= 3 \cdot 10^{-10}$ for CGAUSS(2, 8) and GAUSS4. In such a way, all methods use approximately the same number of mesh points per period (approximately 410) and fixed point iterations (approximately 7.1 per step).[10] Consequently, the cost per period turns out to be comparable for all methods. The three plots in Fig. 2 summarize the errors measured in the computed solution:

- the first plot shows the Hamiltonian error, thus confirming that all the methods are *practically* energy-conserving, with the only exception of GAUSS4, which exhibits a drift in the energy;
- the second plot regards the angular momentum error. A drift for HBVM(8, 2) may be noticed, whereas GAUSS4, GHBVM(8, 2) and CGAUSS(2, 8) are conservative with respect to this invariant;

[10] As a comparison, a fixed stepsize implementation of the methods would require more than 4500 mesh points per period, to obtain the same accuracy.

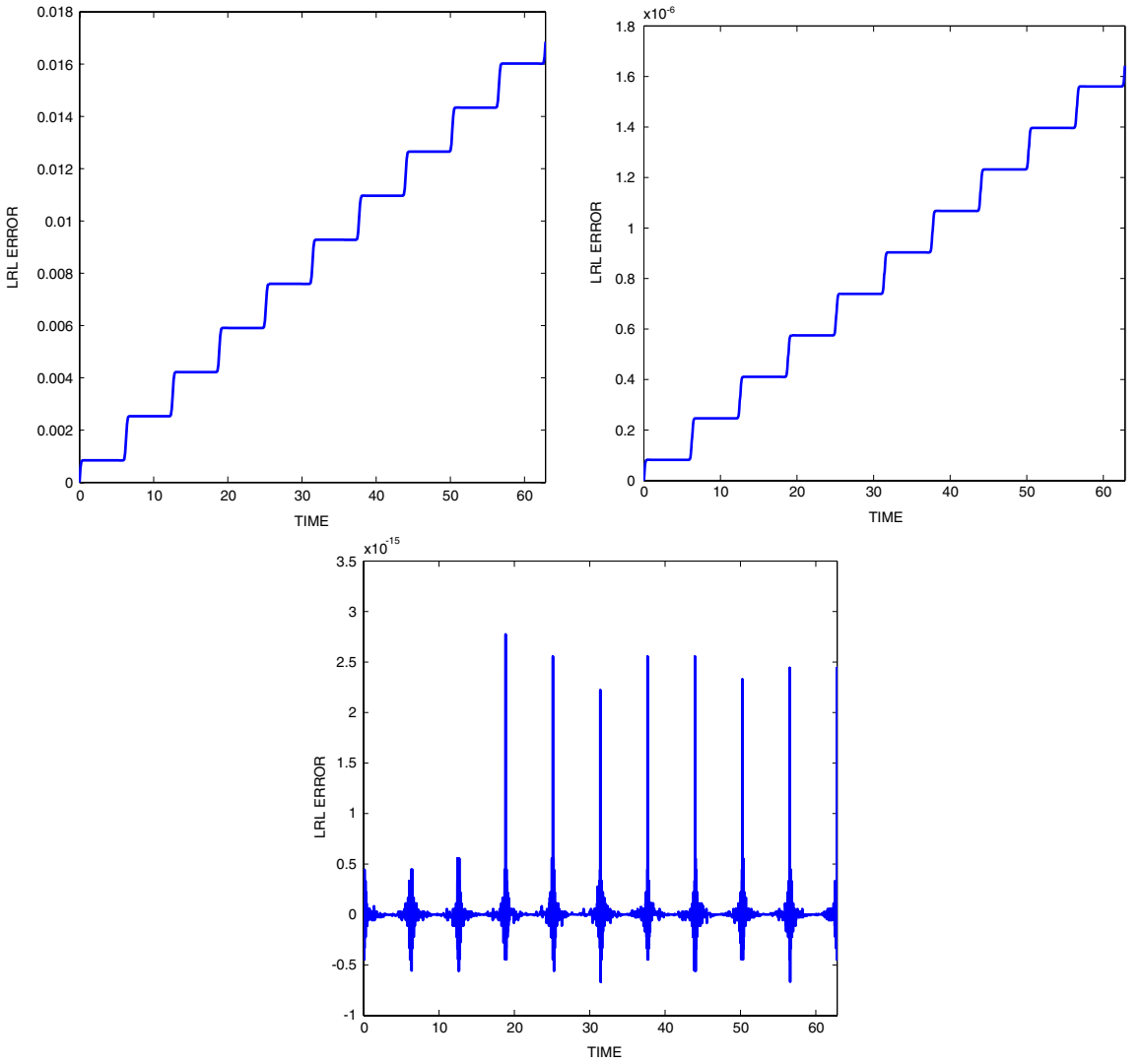

Fig. 3. Errors in the LRL vector (35) by using the fourth-order CGAUSS(2, 8) method with a constant stepsize $h = \pi/50$ and $h = \pi/500$ (first and second plot, respectively) without requiring the explicit conservation of the invariant, and with a constant stepsize $h = \pi/50$ (third plot) by requiring its conservation.

- in the third plot is the error in the computed solution. We see that while GAUSS4 exhibits a quadratic error growth, all the other methods have a comparable error growth, which turns out to be *linear*.

The error estimate for HBVM(8, 2), GHBVM(8, 2), and CGAUSS(2, 8) is obtained by assuming as a reference solution at each step, an approximate solution of the sixth-order HBVM(8, 3) method.[11] This estimate turns out to be inexpensive. In fact, notice that the sixth order method is defined on the very same nodes $\{c_\ell\}$ as each fourth order method. This allows us to use the solution computed by the fourth order method as the initial guess for the fixed point iteration procedure associated with the HBVM(8, 3) method, and a single fixed point iteration is enough to obtain the desired accuracy. For the GAUSS4 method, the error estimate is obtained through the approximate step by GAUSS6. The numerical tests confirm the drift in the angular momentum already observed in [19] for the standard variable stepsize implementation of HBVMs, whereas GHBVM(8, 2) and CGAUSS(2, 8) are still practically angular momentum preserving. On the other hand, it is remarkable to observe the *linear* growth of the solution error for all methods, even using the *standard* mesh selection strategy (34). This, in turn, agrees with the analysis in [25]. The Kepler problem admits a further invariant, namely the Laplace–Runge–Lenz (LRL)

[11] In general, a cheap error estimate for the HBVM(k, r), GHBVM(k, r), and CGAUSS(r, k) methods, can be obtained through an approximate solution of the HBVM$(k, r + 1)$ method.

vector which, for the problem at hand, implies the conservation of the following quantity,

$$F(y) = F(q_1, q_2, p_1, p_2) = q_2 p_1^2 - q_1 p_1 p_2 - \frac{q_2}{\sqrt{q_1^2 + q_2^2}}, \tag{35}$$

besides the energy (32) and the angular momentum (33). However, if we use, for example, the CGAUSS(2, 8) method with a constant stepsize $h = \pi/50$ (with $e = 0.6$) while imposing *only* the conservation of (32) and (33), we find a drift of (35) along the numerical solution, as is shown in the first plot of Fig. 3.[12] Reducing the stepsize to $h = \pi/500$ has only the effect of reducing the amplitude of the drift according to the order of the method, as is shown by the second plot in Fig. 3 (maximum error $1.6 \cdot 10^{-6}$ versus $1.6 \cdot 10^{-2}$). On the other hand, if we impose the conservation of *all* the invariants (32), (33) and (35), the drift disappears, as is shown in the third plot in Fig. 3, where $F(y)$ is evidently conserved up to roundoff errors. Similar results are obtained by using a variable stepsize implementation of the method.

4.2. Example 2

The second test problem that we consider is the Lotka–Volterra problem, i.e., a problem in Poisson form,

$$y' = B(y)\nabla H(y),$$

where $B(y)$ is a skew-symmetric matrix for all y : $B(y)^T = -B(y)$. In such a case, the Hamiltonian is an invariant, as well as its Casimir functions, i.e., scalar functions $C(y)$ such that $\nabla C(y)^T B(y) = 0$, for all y. We consider the problem for which (see [26])

$$B(y) = \begin{pmatrix} 0 & cy_1y_2 & bcy_1y_3 \\ -cy_1y_2 & 0 & -y_2y_3 \\ -bcy_1y_3 & y_2y_3 & 0 \end{pmatrix}, \qquad H(y) = aby_1 + y_2 - ay_3 + \nu \ln y_2 - \mu \ln y_3, \tag{36}$$

and $abc = -1$. It admits the Casimir

$$C(y) = ab \ln y_1 - b \ln y_2 + \ln y_3. \tag{37}$$

We use the same parameters $a = -2$, $b = -1$, $c = -0.5$, $\nu = 1$, $\mu = 2$, and starting point,

$$y(0) = \begin{pmatrix} 1.0 & 1.9 & 0.5 \end{pmatrix}^T, \tag{38}$$

considered in [26]. In such a case, the solution is periodic with period $T \approx 2.878130103817$. We solve this problem by using the CGAUSS(2, 8) method with stepsize $h = T/30 \approx 0.096$, which allows us to measure the error in the computed solution. In particular, we require, in one case, *only* the conservation of the energy $H(y)$ and, in the other case, *both* the conservation of the energy $H(y)$ and of the Casimir $C(y)$. In the former case, one obtains a drift in the Casimir, as is shown in Fig. 4, whereas energy is conserved. In Fig. 5 we plot the error over 100 periods by using the two methods and, as one can see, when only the energy is conserved, then a *quadratic* error growth is observed, whereas it turns out to be *linear*, when both the energy and the Casimir are conserved, again confirming the analysis in [25].

4.3. Example 3

Finally, in order to show the generality of Line Integral Methods for conservative problems, we consider the Lorenz problem,

$$x' = \sigma(y - x), \qquad y' = \rho x - xz - y, \qquad z' = xy - \beta z. \tag{39}$$

When

$$\rho = 0, \qquad \sigma = \frac{1}{2}, \qquad \beta = 1, \tag{40}$$

it admits a constant of motion and two time-variant conserved quantities [27, pp. 5714–5715]

$$H = \frac{y^2 + z^2}{(x^2 - z)^2}, \qquad H_1 = e^t(x^2 - z), \qquad H_2 = e^{2t}(y^2 + z^2). \tag{41}$$

It is evident that H is obtained by eliminating the time between the two time-variant conserved quantities, i.e., $H = H_2/H_1^2$, so that Assumption 1 might not always hold in this case. We solve the problem starting at

$$x(0) = 0.1, \qquad y(0) = 20, \qquad z(0) = 5, \tag{42}$$

[12] It is worth mentioning that a similar result is obtained by using the *symplectic* GAUSS4 method with the same stepsize.

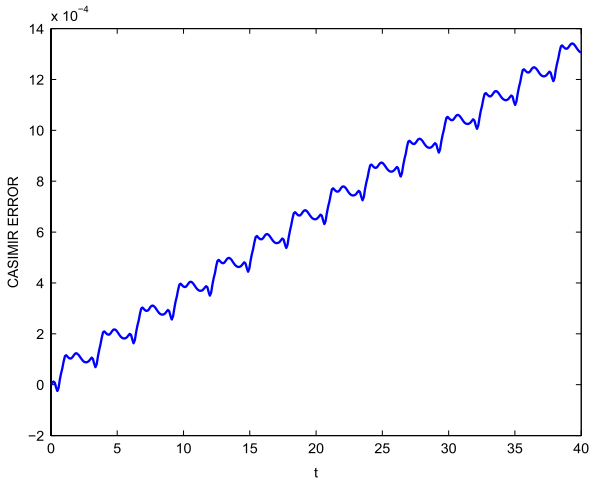

Fig. 4. Drift in the Casimir (37) when solving problem (36)–(38) with the CGAUSS(2, 8) method by requiring *only* energy conservation.

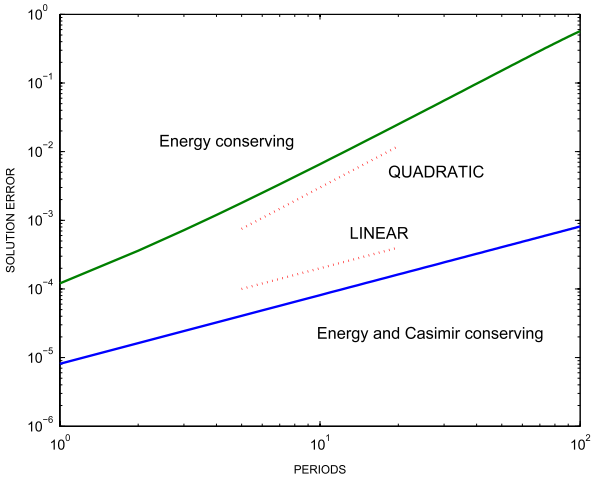

Fig. 5. Errors in the numerical solution over 100 periods when solving problem (36)–(38) with the CGAUSS(2,8) method: a *quadratic* growth is obtained when requiring *only* energy conservation, whereas a *linear* growth is obtained by requiring *both* energy and Casimir conservation.

by using the fourth-order GAUSS4 and CGAUSS(2, 10) methods with a constant stepsize $h = 2.5 \cdot 10^{-2}$, over the interval [0, 10]. The computed numerical solutions (see the upper plot in Fig. 6) differ by at most $4.1 \cdot 10^{-6}$. The overall number of fixed-point iterations for solving the discrete problems is approximately the same for both methods (about 2840). However, the GAUSS4 method has an error in the invariants (41) of the order of $6 \cdot 10^{-7}$, as is shown in the lower-left plot of Fig. 6. Conversely, for the CGAUSS(2, 10) method, for which time has been included in the state in order to require the (practical) conservation of all the invariants, the latter are conserved within roundoff errors, as is confirmed by the lower-right plot in the same figure.

This example clearly shows that *Line Integral Methods* can be conveniently applied for solving *any* kind of conservative problems.

Conclusions

In this paper, we have shown that general conserving methods can be defined for Hamiltonian problems, able to preserve an arbitrary number of invariants, by using the line integral approach, together with its discrete counterpart. This framework defines methods which we collectively call *Line Integral Methods*. A few numerical tests on the Kepler problem show that the possibility of preserving more invariants for the discrete solution results in a more accurate approximation. Moreover, the variable stepsize implementation of these methods can be conveniently done by using a *standard* mesh-selection strategy. Finally, Line Integral Methods can be straightforwardly used for handling any conservative problem, as is confirmed by the numerical tests concerning the Lotka–Volterra problem (cast in Poisson form) and the Lorenz problem.

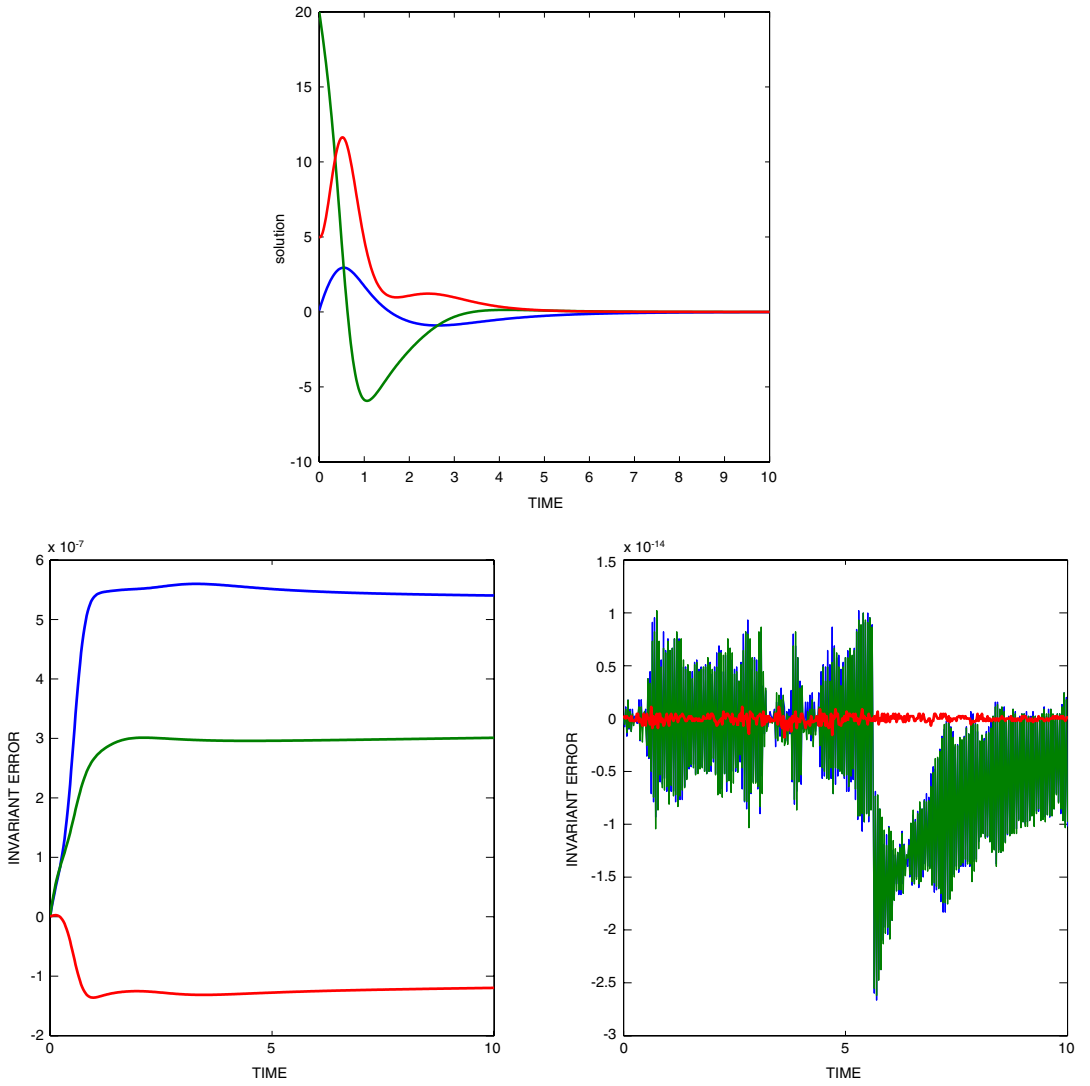

Fig. 6. Lorenz problem (39)–(42) solved by the GAUSS4 and CGAUSS(2, 10) methods, with a constant stepsize $h = 2.5 \cdot 10^{-2}$. Upper plot: numerical solution. Lower plot: relative errors in the invariants (41) for GAUSS4 (left subplot) and CGAUSS(2, 10) (right subplot).

Acknowledgments

Once more, we would like to thank Professor Donato Trigiante for his clear, indefatigable, and insightful guidance during the years, both as a scientist and as a man.

The authors wish to thank the referees for their constructive comments.

References

[1] R.I McLachlan, G.R.W. Quispel, N. Robidoux, Geometric integration using discrete gradient, Philos. Trans. R. Soc. Lond. A Math. Phys. Eng. Sci. 357 (1999) 1021–1045.
[2] F. Iavernaro, B. Pace, *s*-stage trapezoidal methods for the conservation of Hamiltonian functions of polynomial type, AIP Conf. Proc. 936 (2007) 603–606.
[3] F. Iavernaro, B. Pace, Conservative block-boundary value methods for the solution of polynomial Hamiltonian systems, AIP Conf. Proc. 1048 (2008) 888–891.
[4] F. Iavernaro, D. Trigiante, High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems, JNAIAM J. Numer. Anal. Ind. Appl. Math. 4 (1–2) (2009) 87–101.
[5] 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). arXiv:0909.5659 (submitted for publication).
[6] L. Brugnano, F. Iavernaro, D. Trigiante, Hamiltonian BVMs (HBVMs): a family of "drift-free" methods for integrating polynomial Hamiltonian systems, AIP Conf. Proc. 1168 (2009) 715–718.
[7] L. Brugnano, F. Iavernaro, T. Susca, Numerical comparisons between Gauss–Legendre methods and Hamiltonian BVMs defined over Gauss points, Monogr. Acad. Ci. Exact. Fís.-Quím. Nat. Zaragoza 33 (2010) 95–112.

[8] L. Brugnano, F. Iavernaro, D. Trigiante, The Hamiltonian BVMs (HBVMs) homepage. arXiv:1002.2757 (URL: http://www.math.unifi.it/~brugnano/HBVM/).
[9] L. Brugnano, F. Iavernaro, D. Trigiante, Hamiltonian boundary value methods (energy preserving discrete line integral methods), J. Numer. Anal. Ind. Appl. Math. 5 (1–2) (2010) 17–37. arXiv:0910.3621.
[10] L. Brugnano, F. Iavernaro, D. Trigiante, Numerical solution of ODE's and the Columbus' Egg: three simple ideas for three difficult problems, Math. Eng. Sci. Aerosp. 1 (4) (2010) 105–124. arXiv:1008.4789.
[11] L. Brugnano, F. Iavernaro, D. Trigiante, A simple framework for the derivation and analysis of effective classes of one-step methods for ODEs, Appl. Math. Comput. 218 (2012) 8475–8485.
[12] L. Brugnano, F. Iavernaro, D. Trigiante, A note on the efficient implementation of Hamiltonian BVMs, J. Comput. Appl. Math. 236 (2011) 375–383.
[13] E. Hairer, Energy-preserving variant of collocation methods, J. Numer. Anal. Ind. Appl. Math. 5 (1–2) (2010) 73–84.
[14] G.R.W. Quispel, D.I. McLaren, A new class of energy-preserving numerical integration methods, J. Phys. A 41 (2008) 045206. (p. 7).
[15] E. Celledoni, R.I. McLachlan, D. McLaren, B. Owren, G.R.W. Quispel, W.M. Wright, Energy preserving Runge–Kutta methods, M2AN Math. Model. Numer. Anal. 43 (2009) 645–649.
[16] L. Brugnano, F. Iavernaro, D. Trigiante, A two step, fourth-order, method with energy preserving properties, Comput. Phys. Comm. (in press).
[17] L. Brugnano, F. Iavernaro, D. Trigiante, On the existence of energy-preserving symplectic integrators based upon Gauss collocation formulae (2010). arXiv:1005.1930 (submitted for publication).
[18] L. Brugnano, F. Iavernaro, D. Trigiante, Energy and quadratic invariants preserving integrators of Gaussian type, AIP Conf. Proc. 1281 (2010) 227–230. arXiv:1008.4790.
[19] L. Brugnano, F. Iavernaro, D. Trigiante, Numerical comparisons among some methods for Hamiltonian problems, AIP Conf. Proc. 1281 (2010) 214–218. arXiv:1008.4791.
[20] G.R.W. Quispel, H.W. Capel, Solving ODE's numerically while preserving a first integral, Phys. Lett. A 218 (1996) 223–228.
[21] G.R.W. Quispel, H.W. Capel, Solving ODEs numerically while preserving all first integrals, Preprint, 1999.
[22] M. Calvo, D. Hernández-Abreu, J.I. Montijano, L. Rández, On the preservation of invariants by explicit Runge–Kutta methods, SIAM J. Sci. Comput. 28 (3) (2006) 868–885.
[23] L. Brugnano, F. Iavernaro, D. Trigiante, The lack of continuity and the role of infinite and infinitesimal in numerical methods for ODEs: the case of symplecticity, Appl. Math. Comput. 218 (2012) 8053–8063.
[24] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration, second ed., Springer, 2006.
[25] M. Calvo, M.P. Laburta, J.I. Montijano, L. Rández, Error growth in the numerical integration of periodic orbits, Math. Comput. Simulation 81 (2011) 2646–2661.
[26] D. Cohen, E. Hairer, Linear energy-preserving integrators for Poisson systems, BIT 51 (2011) 91–101.
[27] H. Gümral, Y. Nutku, Poisson structure of dynamical systems with three degrees of freedom, J. Math. Phys. 34 (12) (1993) 5691–5723.