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Abstract. A new class of geometric integrators, able to preserve any number of independent invariants of a general conservative problem, is here sketched, by suitably generalizing the line-integral approach which has recently led to the definition of *Hamiltonian BVMs (HBVMs)*, a class of energy-preserving methods for canonical Hamiltonian systems. Because of this reason, the new methods are collectively named *Line Integral Methods*. We here sketch the main results contained in [1].

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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 go back to "discrete gradient methods" (see [15, 18] and references therein). More recently, energy preserving Runge-Kutta methods of order two have been derived in [12], based on the concept of *discrete line integral*. This idea, further developed, has led to fourth order examples of conservative Runge-Kutta methods [13, 14] and, finally, to Hamiltonian Boundary Value Methods (HBVMs) [3, 2, 4, 5, 6, 7, 8], a class of energy-preserving Runge-Kutta methods of any high order. 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. Therefore, it makes sense to devise numerical methods able to preserve a number (possibly all) of them (see also [11]). One successful attempt in this direction has been described in [9, 10], where energy-preserving methods able to preserve also quadratic invariants of canonical Hamiltonian systems are defined and analysed. Additional examples can be found in [16, 17]. We here provide a general framework for this problem, by considering, as a descriptive 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 [1]. The framework is provided by generalizing the *discrete line integral methods* resulting into 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)*, even though the procedure can be naturally extended to *any* discrete method (e.g., collocation methods), whose solution can be suitably associated with a polynomial. With this premise, the paper is organized as follows: at first, the basic facts on HBVMs are recalled; subsequently, LIMs are derived and analysed, in particular, the conservative generalizations of HBVMs; finally, a numerical test is reported which compares the behavior of a few well-known geometrical integrators to that of the new formulae.

HAMILTONIAN BVMS

HBVMs are here recalled by using the approach followed in [5, 6], where it is shown that the methods are related to a local truncated Fourier expansion of the continuous problem. Let then

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

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 $t \geq 0$. By expanding the right-hand side

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of that equation along an orthonormal polynomial basis $\{P_i\}$ on the interval $[0,1]$, one obtains:

$$y'(ch) = \sum_{j\geq 0} \gamma_j(y) P_j(c), \quad c \in [0,1], \qquad \gamma_j(y) = \int_0^1 P_j(\tau) J \nabla H(y(\tau h))\,\mathrm{d}\tau, \quad j \geq 0. \tag{2}$$

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 (2) after r terms, thus obtaining

$$\sigma'(ch) = \sum_{j=0}^{r-1} \gamma_j(\sigma) P_j(c), \qquad c \in [0,1], \qquad \gamma_j(\sigma) = \int_0^1 P_j(\tau) J \nabla H(\sigma(\tau h))\,\mathrm{d}\tau, \quad j \geq 0, \tag{3}$$

whose (polynomial) solution is implicitly defined by $\sigma(ch) = y_0 + h \sum_{j=0}^{r-1} \gamma_j(\sigma) \int_0^c P_j(\tau)\,\mathrm{d}\tau$, $c \in [0,1]$. By using a suitable line integral, one easily realizes that $H(\sigma(h)) = H(y_0)$. In fact,

$$H(\sigma(h)) - H(y_0) = h \int_0^1 \nabla H(\sigma(ch))^T \sigma'(ch)\,\mathrm{d}c = h \sum_{j=0}^{r-1} \gamma_j(\sigma)^T J \gamma_j(\sigma) = 0, \tag{4}$$

considering that matrix J is skew-symmetric. Furthermore, the following result can be proved (see, e.g., [6]).

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

We use a quadrature formula defined at the abscissae $\{c_1, \ldots, c_k\}$, having order of accuracy q (that is, exact for polynomials of degree at least $q-1$), to approximate the integrals appearing in (3). One then obtains

$$u'(ch) = \sum_{j=0}^{r-1} P_j(c) \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f(u(c_\ell)). \tag{5}$$

Hereafter, we shall consider a Gaussian quadrature formula, so that $q = 2k$. Equation (5) 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 $2r$ [4] (for completeness, we also mention that HBVMs defined at Lobatto nodes were previously considered in [3]). Consequenly, one obtains that $\sigma \equiv u$ in the case where H is a polynomial of degree no larger than $2k/r$. Otherwise, the two polynomials will differ. However, by choosing k large enough, a *practical* conservation of energy can be always obtained. Indeed, the following result hold true (see, e.g., [6]).

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

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 invariant of the continuous dynamical system. For sake of brevity, we shall only discuss the case of two invariants (e.g., the Hamiltonian $H(y)$ and another one, say $L(y)$), 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 the dynamical system induced by (1) admits a (smooth) invariant $L(y)$ if and only if, along any trajectory $y(t)$, and for any $h > 0$, $L(y(h)) - L(y_0) = h \int_0^1 \nabla L(y(\tau h))^T y'(\tau h)\,\mathrm{d}\tau = h \sum_{j\geq 0} \phi_j(y)^T \gamma_j(y) = 0$, where we have used the expansion (2) and the following one: $\nabla L(y(ch)) = \sum_{j\geq 0} P_j(c) \int_0^1 P_j(\tau) \nabla L(y(\tau h))\,\mathrm{d}\tau \equiv \sum_{j\geq 0} P_j(c) \phi_j(y)$, $c \in [0,1]$. Moreover, we shall denote by $\{\rho_j(y)\}_{j\geq 0}$ the Fourier coefficients of $\nabla H(y)$, namely $\rho_j(y) = J^T \gamma_j(y)$. With this premise, the variant of HBVMs able to preserve *both* the invariants, is defined by the formula

$$\sigma'(ch) = \sum_{j=0}^{r-1} P_j(c) \gamma_j(\sigma) \; + \; P_0(c) \left(x_1 \rho_0(\sigma) + x_2 \phi_0(\sigma) \right), \qquad c \in [0,1], \tag{6}$$

in place of (3). The coefficients x_1, x_2 are then chosen in order to obtain the conservation conditions $H(\sigma(h)) = H(y_0)$ and $L(\sigma(h)) = L(y_0)$. Under mild assumptions, this can be always achieved, thus obtaining that Theorem 1 continues formally to hold (we refer to [1] for full details). The discretization issue then proceeds as for the previous case, by approximating the integrals defining the Fourier coefficients by a suitable quadrature rule at the abscissae $\{c_1, \ldots, c_k\}$. The resulting polynomial approximation, say $u(ch)$, still satisfies Theorem 2 for any invariant, besides $H(y)$, when the k abscissae are placed at the Gauss points on $[0,1]$: this conservative method will be referred to as GHBVM(k,r).

A NUMERICAL TEST

The Kepler problem, defined by the Hamiltonian function $H(y) \equiv H(q_1,q_2,p_1,p_2) = \frac{1}{2}\left(p_1^2+p_2^2\right) - \left(q_1^2+q_2^2\right)^{-\frac{1}{2}}$, admits three independent first integrals: the Hamiltonian itself, the total angular momentum, $M(y) \equiv L(q_1,q_2,p_1,p_2) = q_1p_2 - q_2p_1$, and the Laplace-Runge-Lenz (LRL) vector, $A(y) \equiv A(q_1,q_2,p_1,p_2) = q_2p_1^2 - q_1p_1p_2 - q_2\left(q_1^2+q_2^2\right)^{-\frac{1}{2}}$. Since the phase space has dimension four, any integrator that preserves all these invariants has the property to generate a discrete orbit that lies on the very same continuous orbit (an ellipse) of the original problem.

The aim of the present test is to compare a few geometrical integrators on the basis of their qualitative properties in reproducing a consistent phase portrait. In particular, since for h small all the integrators we use would produce good results, we are interested in using an as large as possible stepsize h and see how the choice of h affects the stability properties of the corresponding numerical solution.

We consider the following methods of order four: GHBVM(10,2) described above, which yields a conservation of the three first integrals within machine precision; the energy-conserving method HBVM(10,2), and the (symplectic) Gauss method of order four (GAUSS4). For comparison reasons we also consider the Symplectic Euler method and the Störmer–Verlet method.

We first integrate the problem on the time interval $[0,300]$, with stepsize $h = 0.03$ and initial condition $y_0 = [\frac{1}{10}, 0, 0, \sqrt{\frac{1.9}{0.1}}]^T$ which yields an ellipse with eccentricity $e = 0.9$ and major-axis $d = 2$. As is clear from the left picture of Figure 1 the GHBVM(10,2) faithfully reproduces such an ellipse in the (q_1,q_2)-plane. The HBVM(10,2) introduces a sham rotation of the plane but does not deform the shape of the ellipse. This is also deduced from the right picture of Figure 1 that reports the distance of the moving point from the focus located at the origin O: the oscillations produced by the HBVM are uniform and there is no relevant difference from the analogous plot for the GHBVM. On the contrary, the solution produced by GAUSS4, though bounded (at least on the selected time window), displays an irregular behaviour and the ellipse, while rotating, undergoes repentine deformations (see the bottom-right plot).

Finally, we compute the average major axes of the elliptical shaped orbits, and display the corresponding absolute error as a function of the stepsize $h \in [0.001, 0.05]$ (see Figure 2). The two explicit methods evidently have poorer stability properties if compared to the three implicit methods: they tend to strongly enlarge the theoretical ellipse and the numerical solutions they provide become unbounded for moderate values of the stepsize h (the two lines break for values of h as larger as 0.02). The solution provided by GAUSS4 is unbounded for h larger than 0.035 and, before that critical value, yields oscillations that differ significantly from the original ones in amplitude. The HBVM and the GHBVM produce comparable results: since we have considered the same integration interval independently of h, a moderate growth of the error is rightly expected as h increases, due to the numerical procedures that approximate the ellipses enveloping the numerical orbit at each oscillation around the focus.

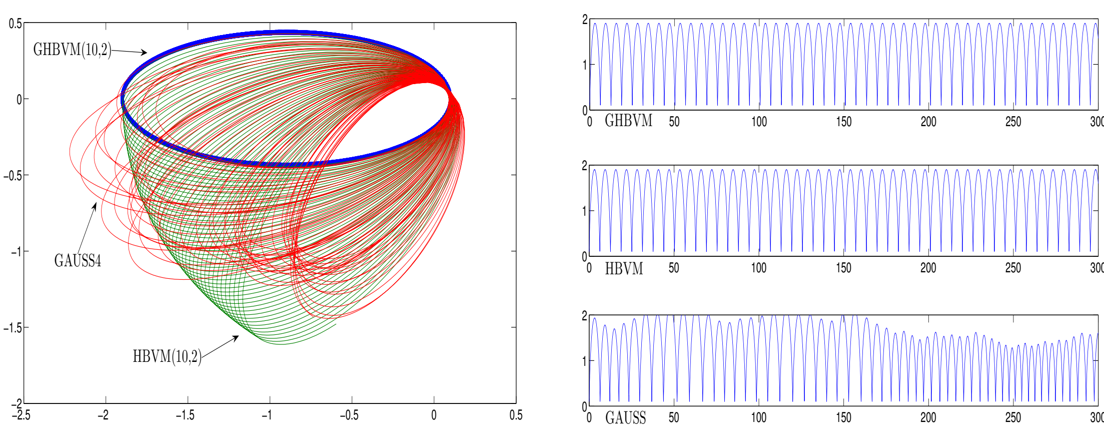

FIGURE 1.

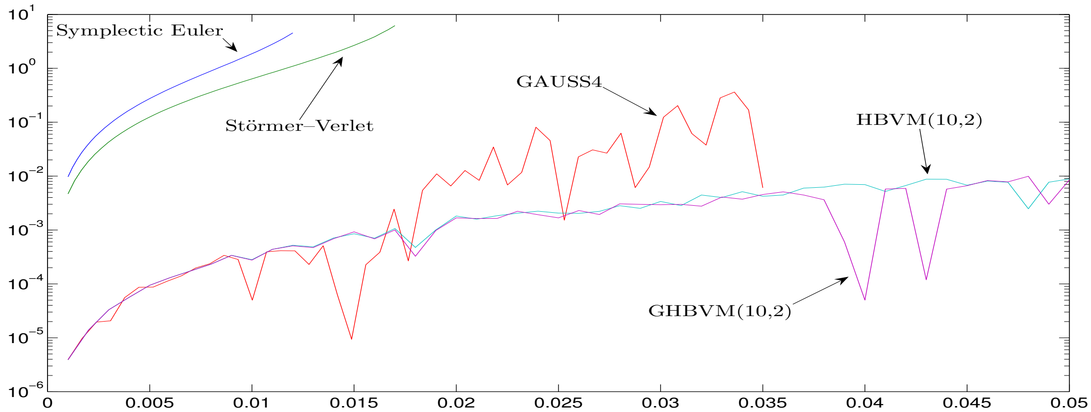

FIGURE 2.

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