Hamiltonian BVMs (HBVMs): a family of “drift free” methods for integrating polynomial Hamiltonian problems[1]

Luigi Brugnano[*], Felice Iavernaro[†] and Donato Trigiante[**]

[*]*Dipartimento di Matematica “U. Dini”, Viale Morgagni 67/A, 50134 Firenze, Italy.*
[†]*Dipartimento di Matematica, Via Orabona 4, 70125 Bari, Italy.*
[**]*Dipartimento di Energetica “S. Stecco”, Via Lombroso 6/17, 50134 Firenze, Italy.*

Abstract. In this paper, we present a number of numerical results concerning the newly introduced class of *Hamiltonian Boundary Value Methods* (hereafter, *HBVMs*). Such methods are very suited for the numerical integration of Hamiltonian problems, since they are able to preserve, in the discrete solution, the exact value of polynomial Hamiltonians. In such a way, a numerical drift of the Hamiltonian, sometimes experienced when solving such problems, cannot occur.

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INTRODUCTION

Let

$$y' = J\nabla H(y), \qquad y(0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

be a Hamiltonian problem, where

$$J = \begin{pmatrix} & I_m \\ -I_m & \end{pmatrix}, \quad \text{with } I_m \text{ the identity matrix of dimension } m, \tag{2}$$

and where the Hamiltonian function, $H(y)$, is a polynomial of degree ν. One has that, over a trajectory, $y(t)$, of (1)

$$H(y(t)) = H(y_0) + \int_0^t \nabla H(y(\tau))^T y'(\tau)d\tau = H(y_0) + \int_0^t \nabla H(y(\tau))^T J\nabla H(y(\tau))d\tau = H(y_0), \tag{3}$$

due to the fact that matrix J in (2) is skew-symmetric. More in general, from the conservative nature of the vector field it follows that

$$H(y^*) - H(y_0) = \int_{y_0\to y^*} \nabla H(y)^T dy = h\int_0^1 \sigma'(t)^T \nabla H(\sigma(t))dt, \tag{4}$$

where $\sigma : [0,1] \to R^{2m}$ is any smooth curve such that

$$\sigma(0) = y_0, \qquad \sigma(1) = y^*.$$

In particular, we here consider the case where $\sigma(t)$ is a polynomial of degree s, which interpolates the solution of problem (1)[2] at the abscissae

$$0 = c_0 < c_1 < \ldots < c_s = 1, \tag{5}$$

i.e., one has:[3]

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[1] Work developed within the project “Numerical methods and software for differential equations”.
[2] Actually, it is an approximate solution of the problem.
[3] The polynomial σ is not a collocation polynomial, even though it is related to it.

$$\sigma(c_i) = y_i, \qquad i = 0,\dots,s. \tag{6}$$

Let us now approximate the integral in (4) by means of a quadrature formula, with knots (5) and weights

$$b_i = \int_0^1 \prod_{j=0,\, j\neq i}^{s} \frac{t-c_j}{c_i-c_j}dt, \qquad i = 0,1,\dots,s, \tag{7}$$

which has degree of precision ranging from s to $2s-1$, depending on the choice of the abscissae (5). In particular, the highest precision degree is obtained by using the Lobatto abscissae, which we shall consider in the sequel. [4] We now ask for preserving the Hamiltonian function $H(y)$ at the end-point of the discrete trajectory. From (4) we require then that

$$\int_0^1 \sigma'(t)^T \nabla H(\sigma(t))dt = \sum_{i=0}^{s} b_i \sigma'(c_i)^T \nabla H(\sigma(c_i)) = 0, \tag{8}$$

i.e., that the quadrature formula is exact when applied to the given function, and that the integral itself vanishes. However, since the integrand has degree

$$(s-1)+(\nu-1)s = \nu s - 1,$$

it follows that the maximum allowed value for ν is 2. Indeed, it is well known that quadratic invariants are preserved by symmetric collocation methods. For the general case, one would need a quadrature formula with, say, $k+1$ points, where

$$k = \left\lceil \frac{\nu s}{2} \right\rceil, \tag{9}$$

if the corresponding Lobatto abscissae are used. For this purpose, let $r = k-s$ be the number of the required additional points, and let

$$0 < \tau_1 < \ldots < \tau_r < 1, \tag{10}$$

be r additional abscissae distinct from (5). Moreover, let us define the following *silent stages* [11]

$$w_i \equiv \sigma(\tau_i), \qquad i = 1,\dots,r. \tag{11}$$

Consequently, the polynomial $\sigma(t)$, which interpolates the couples (c_i, y_i), $i = 0,1,\dots,s$, also interpolates the couples (τ_i, w_i), $i = 1,\dots,r$. That is, $\sigma(t)$ interpolates at $k+1$ points, even though it has only degree s. Consequently, if we define the following abscissae,

$$\{t_0 < t_1 < \ldots < t_k\} = \{c_i\} \cup \{\tau_i\}, \tag{12}$$

which will coincide with the Lobatto abscissae of the formula of degree $2k$,[5] one obtains that

$$\int_0^1 \sigma'(t)^T \nabla H(\sigma(t))dt = \sum_{i=0}^{k} b_i \sigma'(t_i)^T \nabla H(\sigma(t_i)), \tag{13}$$

where, now,

$$b_i = \int_0^1 \prod_{j=0,\, j\neq i}^{k} \frac{t-t_j}{t_i-t_j}dt, \qquad i = 0,1,\dots,k. \tag{14}$$

Imposing that the sum in (13) vanish, allows us to derive methods, called *Hamiltonian Boundary Value Methods (HBVMs)* [2], which have order $2s$ for all $s = 1,2,\ldots$, and are able to exactly preserve polynomial Hamiltonians of degree k (see (9)). In particular, when $k = s$ (i.e., in the case of a quadratic Hamiltonian), one obtains the Lobatto

[4] Different choices of the abscissae will be the subject of future investigations.
[5] More general choices of the abscissae will be the subject of future investigations.

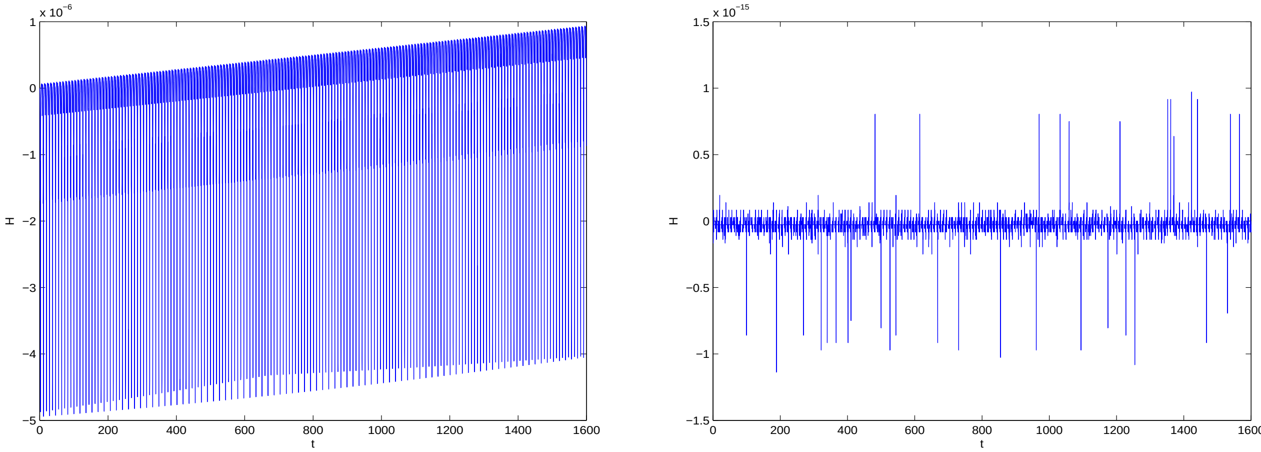

FIGURE 1. Problem (15): fourth-order Lobatto IIIA method (left picture), and HBVM(6,2) (right picture), $h = 0.16$.

IIIA methods. Moreover, a practical preservation of the Hamiltonian over the numerical solution can be achieved also in the case of a non-polynomial Hamiltonian since, under suitable regularity assumptions, the latter can be locally approximated, to machine precision, by a polynomial of sufficiently high degree.

NUMERICAL TESTS

The actual cost for implementing the HBVM(k,s) methods above described, can be seen to depend on s, rather than on k. However, we here skip such details, which will be described in a future paper [3] and sketched in [1]. Instead, we here report a few numerical tests, in order to show the potentialities of such methods.

Let then consider, at first, the Hamiltonian problem characterized by the polynomial Hamiltonian (4.1) in [6],

$$H(p,q) = \frac{p^3}{3} - \frac{p}{2} + \frac{q^6}{30} + \frac{q^4}{4} - \frac{q^3}{3} + \frac{1}{6}, \tag{15}$$

having degree $\nu = 6$, starting at the initial point $y_0 \equiv (q(0), p(0))^T = (0,1)^T$. For such a problem, in [6] it is experienced a numerical drift in the discrete Hamiltonian, when using the fourth-order Lobatto IIIA method[6] with stepsize $h = 0.16$. This is confirmed by the left plot in Figure 1, where a linear drift in the numerical Hamiltonian is evident. On the other hand, by using the fourth-order HBVM(6,2) method with the same stepsize, the drift disappears, as it is shown in the right plot in Figure 1, since such method exactly preserves polynomial Hamiltonians of degree 6.

The second test problem is the Fermi-Pasta-Ulam problem [7, Section I.5.1], defined by the Hamiltonian

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\sum_{i=1}^{m}\left(p_{2i-1}^2 + p_{2i}^2\right) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4, \tag{16}$$

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

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

In such a case, the Hamiltonian function is a polynomial of degree 4, so that the fourth-order HBVM(4,2) method, which is used with stepsize $h = 0.05$, is able to exactly preserve the Hamiltonian, as confirmed by the right plot in Figure 2, whereas the fourth-order Lobatto IIIA method provides the result plotted in the left plot in the same figure.

Finally, in the following tables we list the measured numerical order of convergence for the HBVM(6,2) method on problem (15) and for the HBVM(4,2) method on problem (16), respectively, which confirm their fourth-order accuracy.

[6] which coincides with the HBVM(2,2) above described.

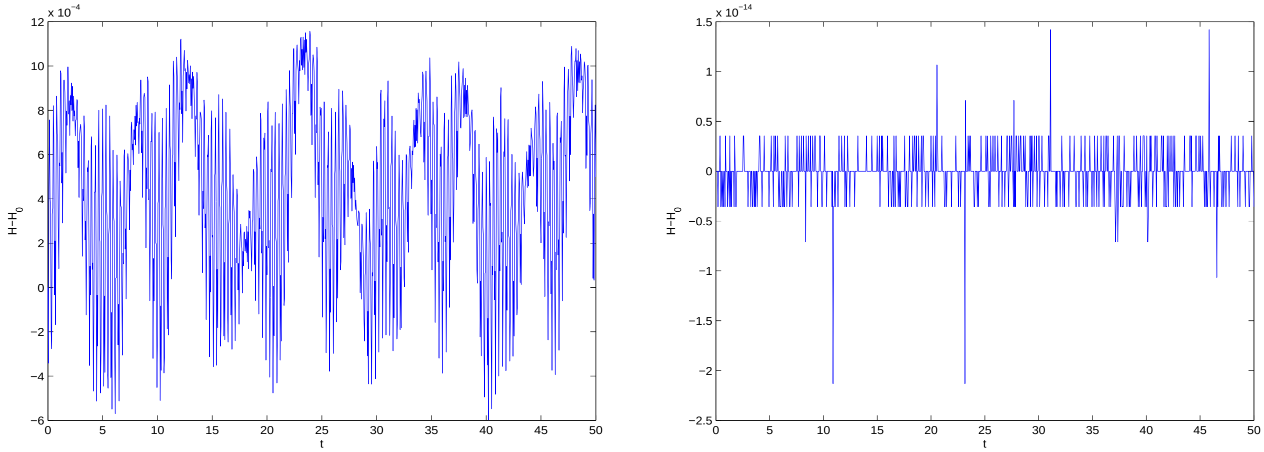

FIGURE 2. Problem (16): fourth-order Lobatto IIIA method (left picture) and HBVM(4,2) (right picture), $h = 0.05$.

h	0.32	0.16	0.08	0.04	0.02
error	$2.288 \cdot 10^{-2}$	$1.487 \cdot 10^{-3}$	$9.398 \cdot 10^{-5}$	$5.890 \cdot 10^{-6}$	$3.684 \cdot 10^{-7}$
order	–	3.94	3.98	4.00	4.00

h	$1.6 \cdot 10^{-2}$	$8 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	$2 \cdot 10^{-3}$	10^{-3}
error	3.030	$1.967 \cdot 10^{-1}$	$1.240 \cdot 10^{-2}$	$7.761 \cdot 10^{-4}$	$4.853 \cdot 10^{-5}$
order	–	3.97	3.99	4.00	4.00

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