Hamiltonian BVMs (HBVMs): implementation details and applications[1]

Luigi Brugnano*, Felice Iavernaro† and Tiziana Susca†

*Dipartimento di Matematica "U. Dini", Viale Morgagni 67/A, 50134 Firenze, Italy.
†Dipartimento di Matematica, Via Orabona 4, 70125 Bari, Italy.

Abstract. Hamiltonian Boundary Value Methods are one step schemes of high order where the internal stages are partly exploited to impose the order conditions (*fundamental stages*) and partly to confer the formula the property of conserving the Hamiltonian function when this is a polynomial with a given degree ν. The term "*silent stages*" has been coined for these latter set of extra-stages to mean that their presence does not cause an increase of the dimension of the associated nonlinear system to be solved at each step. By considering a specific method in this class, we give some details about how the solution of the nonlinear system may be conveniently carried out and how to compensate the effect of roundoff errors.

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INTRODUCTION

A Hamiltonian system with m degrees of freedom takes the form

$$\begin{cases} \dot{y} = J\nabla H(y), \\ y(t_0) = y_0, \end{cases} \qquad J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix}, \tag{1}$$

(I_m is the identity matrix of dimension m). The state vector y splits into two m-length vectors p and q, the conjugate momenta and the generalized coordinates, respectively.

Its study deserves a huge interest in many application and research fields, where it is used to model specific evolutionary problems where one or a number of functions depending on the state variables (the *first integrals*) remain constant while the system evolves. Among such functions, one of the most important is the Hamiltonian function itself $H(y)$, sometimes referred to as *Energy function*. The numerical integration of problem (1) is a very delicate issue to handle because, in general, the method destroys two peculiar properties of such systems: the conservation of the Hamiltonian function and the symplecticity of the associated flow. While many classes of numerical methods have been devised in the past years, which preserve this latter property, weaker results are available in the literature concerning the former question. For example, it is well known that a symplectic method only conserve quadratic Hamiltonian functions[2] [6] and, on the other hand, energy conserving methods (such as discrete gradient methods) have low order.

More recently [9, 7, 8, 2], high order one step schemes $y_n = \Phi_h(y_{n-1})$ have been introduced, capable of providing numerical approximations y_n to the true solution $y(t_n)$ such that

$$H(y_{n+1}) = H(y_n), \qquad \text{for all } n \text{ and } h > 0, \tag{2}$$

in the case where $H(p,q)$ is a polynomial of degree ν, in the variables p and q. Such formulae are more naturally devised in the class of block-Boundary Value Methods (block-BVMs), and therefore they take the form

$$(A \otimes I)Y - h\big(B \otimes J\big)\nabla H(Y) = -a_0 \otimes y_0 + hb_0 \otimes J\nabla H(y_0), \tag{3}$$

[1] Work developed within the project "Numerical methods and software for differential equations".
[2] A drift of the Energy function is experienced by most of the standard methods, see for example [5, 4].

where

$$Y \equiv \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{pmatrix}, \qquad \nabla H(Y) \equiv \begin{pmatrix} \nabla H(y_1) \\ \nabla H(y_2) \\ \vdots \\ \nabla H(y_k) \end{pmatrix},$$

I is the identity matrix of dimension $2m$, while the two k vectors a_0 and b_0 and the $k \times k$ matrices A and B contain the coefficients that form the linear combination of the vectors y_i and $J\nabla H(y_i)$ respectively. System (3) represents the standard form of a block-BVM (refer to [3] for the general theory on Boundary Value Methods). The vector stages y_i, $i = 1,\ldots,k$, approximate the true solution at the given times $t_i = t_0 + c_i h$, where $0 = c_0 < c_1 < \ldots < c_k = 1$ are the associated abscissae. The trick to achieve (2) is to use the k stages y_i partly to confer the method a given order (*fundamental stages*), and partly to accomplish a number of orthogonality conditions (*silent stages*) (see [2, 9] for details) which guarantee formula (2) to be satisfied. The deriving methods are called Hamiltonian Boundary Value Methods (HBVMs in the sequel). The number, say $s+1$, of fundamental stages solely depends on the order of the method, while the number, say $r = k - s$, of silent stages solely depends on the degree ν of the Hamiltonian of the problem. By using a Lobatto distribution of the abscissae c_i, both the order of the method and its degree of precision ν are maximized: in particular the order is $2s$, while $\nu = \lfloor 2\left(1 + \frac{r}{s}\right)\rfloor$. As an instance, to $s = 2$ and $r = 4$ there corresponds a HBVM of order 4 and capable to conserve Hamiltonian functions of degree less than or equal to 6. Such a method has been successfully used in [1] to integrate a polynomial problem of degree 6 which causes a drift in the energy function for several well known symmetric/symplectic methods. Written as a Runge-Kutta method, its explicit expression has been reported in Table 1. Hereafter we use this specific method as a practical example to sketch how the implementation of HBVMs may be conveniently carried out.

IMPLEMENTING HBVMS

To each HBVM it is possible to associate an underlying *extended* collocation polynomial $\sigma(c)$ which has degree s [9]. The term "extended" has been used to stress that although $\sigma(c_i) = y_i$, for $i = 0,\ldots,k$, the polynomial σ fails to satisfy the collocation conditions $\sigma'(c_i) = f(\sigma(c_i))$ (in [2] the relation between $\sigma(c)$ and the classical collocation polynomial $u(c)$ is elucidated). Denoting by $\mathscr{I}_1$ and $\mathscr{I}_2$ the sets of indices corresponding to the fundamental and silent stages respectively, it follows that $\sigma(c)$ is uniquely identified by the $s+1$ interpolation conditions $\sigma(c_j) = y_j$, $j \in \mathscr{I}_1$. Therefore all silent stages turn out to be a linear combination of fundamental stages, according to the formula

$$y_j = \sigma(c_j), \qquad \text{for} \quad j \in \mathscr{I}_2. \tag{4}$$

Each of the r equations (4) represents a linear multistep formula involving the fundamental stages and a single silent stage; in particular we note that in (4) there is no explicit trace of the nonlinear function $H(y)$. Such equations will be inserted as components of the nonlinear vector equation (3) that must be solved to advance the solution. As a consequence, the $k \times k$ matrix B in (3) will count r null rows, that we assume as the last ones. Inserting in (3) the UL factorization of the matrix A yields

$$(L \otimes I)Y - h\big(U^{-1}B \otimes J\big)\nabla H(Y) = -U^{-1}a_0 \otimes y_0 + hU^{-1}b_0 \otimes J\nabla H(y_0). \tag{5}$$

The matrix $U^{-1}B$ has still null all the entries in the last r rows, which allows us to easily split in (5) the linear and nonlinear part.

A similar argument may be also exploited when the HBVM is recast in Runge-Kutta notation: hereafter we concentrate our attention to this last form and, in particular, to the method in Table 1, in order to better emphasize a noticeable property that links the present family of HBVMs to the family of Lobatto IIIA methods to which they reduce when $r = 0$. Written as Runge Kutta method, (3) takes the form

$$\widehat{Y} = e \otimes y_0 + h \begin{pmatrix} 0 \ldots\ldots 0 \\ A^{-1}[b_0|B] \end{pmatrix} \otimes J\nabla H(\widehat{Y}). \tag{6}$$

with $\widehat{Y} = [y_0^T, Y^T]^T$ and $e = [1,\ldots,1]^T$. Due to the structure of B, the $(k+1) \times (k+1)$ matrix in (6) has rank $s = 2$. More precisely, a direct computation shows that the two non-null eigenvalues are $\frac{1}{4} \pm i\frac{1}{12}\sqrt{3}$, the same as the matrix associated to the LOBATTO IIIA method of order 4. This circumstance, which holds true for any choice of s and k,

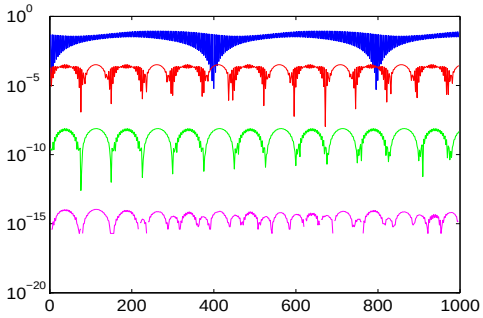
reveals the link between a HBVM and the corresponding generating Lobatto formula: a change of variables of the form $\widehat{Z} = (T^{-1} \otimes I)\widehat{Y}$ exists such that (6) may be recast as

$$\widehat{Z} = \hat{e} \otimes y_0 + h \begin{pmatrix} 0 & \\ & A_{\text{LOB}} \end{pmatrix} \otimes JG(\widehat{Z}), \tag{7}$$

where $\hat{e} = T^{-1}e$, $G(\widehat{Z}) = (T^{-1} \otimes I)\nabla H((T \otimes I)\widehat{Z})$ and A_{LOB} is the matrix associated to the LOBATTO IIIA method of order 4. Since the first row of A_{LOB} is indeed null, the first 5 block components of $\widehat{Z}$ coincide with the corresponding ones in the vector $\hat{e} \otimes y_0$, while the remaining two components are retrieved by solving a complex nonlinear system of dimension $2m$. In conclusion, since the multiplication $(T \otimes I)\widehat{Z}$ requires only $k^2 m$ multiplications, the bulk of the computational cost for the solution of the nonlinear system is not heavily influenced by the number r of the silent stages introduced and is comparable to that of the underlying Lobatto formula[3].

Another practical aspect to mention is that the use of finite arithmetic causes the numerical solution to satisfy the conservation relation (2) up to the machine precision times the conditioning number of the nonlinear system that is to be solved at each step. To prevent the accumulation of roundoff errors we apply a simple and costless *correction* technique on the approximation y_k which consists in a single step of a gradient descent method. More precisely the correction y_n^* is defined by $y_n^* = y_n - \alpha \frac{\nabla H(y_n)}{||\nabla H(y_n)||_2}$ where the scalar α is obtained by the minimization of the linear part of the scalar function $\Phi(\alpha) = H(y_n - \alpha \frac{\nabla H(y_n))}{||\nabla H(y_n)||_2}) - H(y_0)$ and therefore assumes the value $\alpha = \frac{H(y) - H(y_0)}{||\nabla H(y_n)||_2}$.

To conclude, we consider a non-polynomial Hamiltonian problem, namely the nonlinear pendulum equation defined by $H(p,q) = \frac{1}{2}p^2 + 1 - cos(q)$, and solve it by means of the HBVM of order 2 for several increasing values of r. The aim is to show that HBVMs can provide a *practical conservation* of the Hamiltonian function even when $H(y)$ is not a polynomial. This is easily understood after observing that the HBVM precisely conserve the Hamiltonian function of a polynomial that, under suitable smoothness assumptions, approximate $H(y)$ better and better as long as we increase the number of silent stages (see [9] for details). This situation is evident in the picture where we have reported the relative errors $|H(y_n) - H(y_0)|/|H(y_0)|$ of the numerical Hamiltonian function related to the application of the four HBVMs of order 2 corresponding to the choices $r = 0, 1, 3, 5$ (from the top to the bottom) , with stepsize $h = 1$, number of points $n = 1000$ and initial condition $[p_0, q_0] = [1/2, \pi/2]$.



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[3] The cost of the LU factorization of a complex system of dimension $2m$ is $32m^3/3$ multiplications.

1: The Butcher tableau of the HBVM with order 4 and degree of precision 6, written in Runge Kutta notation. Four of the 7 stages are *silent*, which means that the underlying nonlinear system to be solved has the same dimension as the Lobatto IIIA method of order 4 (see section 2 for details).

c_0	0	0	0	0	0	0	0
c_1	$-\frac{1}{924}\sqrt{15}+\frac{5}{231}$ $+\frac{1}{7623}\eta_1-\frac{5}{30492}\eta_2$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $-\frac{3}{7700}\eta_1+\frac{1}{9240}\eta_2$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $-\frac{919}{508200}\eta_1-\frac{373}{254100}\eta_2$ $+\frac{337}{169400}\eta_3-\frac{61}{169400}\eta_4$	$\frac{64}{525}-\frac{1184}{190575}\eta_1+\frac{32}{38115}\eta_2$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $-\frac{919}{508200}\eta_1-\frac{373}{254100}\eta_2$ $-\frac{337}{169400}\eta_3+\frac{61}{169400}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $-\frac{2}{385}\eta_1+\frac{107}{46200}\eta_2$	$\frac{1}{462}+\frac{1}{924}\sqrt{15}$ $+\frac{1}{7623}\eta_1-\frac{5}{30492}\eta_2$
c_2	$\frac{5}{231}+\frac{1}{924}\sqrt{15}$ $+\frac{1}{7623}\eta_3+\frac{5}{30492}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $+\frac{337}{169400}\eta_1+\frac{61}{169400}\eta_2$ $-\frac{919}{508200}\eta_3-\frac{373}{254100}\eta_4$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $-\frac{3}{7700}\eta_3-\frac{1}{9240}\eta_4$	$\frac{64}{525}-\frac{1184}{190575}\eta_3-\frac{32}{38115}\eta_4$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $-\frac{2}{385}\eta_3-\frac{107}{46200}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $-\frac{337}{169400}\eta_1-\frac{61}{169400}\eta_2$ $-\frac{919}{508200}\eta_3+\frac{373}{254100}\eta_4$	$\frac{1}{462}-\frac{1}{924}\sqrt{15}$ $+\frac{1}{7623}\eta_3+\frac{5}{30492}\eta_4$
c_3	$\frac{5}{168}$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $+\frac{31}{7700}\eta_1-\frac{3}{4400}\eta_2$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}+\frac{31}{7700}\eta_3+\frac{3}{4400}\eta_4$	$\frac{64}{525}$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}-\frac{31}{7700}\eta_3-\frac{3}{4400}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}-\frac{31}{7700}\eta_1+\frac{3}{4400}\eta_2$	$-\frac{1}{168}$
c_4	$\frac{5}{231}+\frac{1}{924}\sqrt{15}$ $-\frac{1}{7623}\eta_3-\frac{5}{30492}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $+\frac{337}{169400}\eta_1+\frac{61}{169400}\eta_2$ $+\frac{919}{508200}\eta_3-\frac{373}{254100}\eta_4$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $+\frac{2}{385}\eta_3+\frac{107}{46200}\eta_4$	$\frac{64}{525}+\frac{1184}{190575}\eta_3+\frac{32}{38115}\eta_4$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $+\frac{3}{7700}\eta_3+\frac{1}{9240}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $-\frac{337}{169400}\eta_1-\frac{61}{169400}\eta_2$ $+\frac{919}{508200}\eta_3-\frac{373}{254100}\eta_4$	$\frac{1}{462}-\frac{1}{924}\sqrt{15}$ $-\frac{1}{7623}\eta_3-\frac{5}{30492}\eta_4$
c_5	$\frac{5}{231}-\frac{1}{924}\sqrt{15}$ $-\frac{1}{7623}\eta_1+\frac{5}{30492}\eta_2$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $+\frac{2}{385}\eta_1-\frac{107}{46200}\eta_2$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $+\frac{919}{508200}\eta_1+\frac{373}{254100}\eta_2$ $+\frac{337}{169400}\eta_3-\frac{61}{169400}\eta_4$	$\frac{64}{525}+\frac{1184}{190575}\eta_1-\frac{32}{38115}\eta_2$	$\frac{31}{350}+\frac{1}{200}\sqrt{15}$ $+\frac{919}{508200}\eta_1+\frac{373}{254100}\eta_2$ $-\frac{337}{169400}\eta_3+\frac{61}{169400}\eta_4$	$\frac{31}{350}-\frac{1}{200}\sqrt{15}$ $+\frac{3}{7700}\eta_1-\frac{1}{9240}\eta_2$	$\frac{1}{462}+\frac{1}{924}\sqrt{15}$ $-\frac{1}{7623}\eta_1+\frac{5}{30492}\eta_2$
c_6	$\frac{1}{42}$	$\frac{31}{175}-\frac{1}{100}\sqrt{15}$	$\frac{31}{175}+\frac{1}{100}\sqrt{15}$	$\frac{128}{525}$	$\frac{31}{175}+\frac{1}{100}\sqrt{15}$	$\frac{31}{175}-\frac{1}{100}\sqrt{15}$	$\frac{1}{42}$
	$\frac{1}{42}$	$\frac{31}{175}-\frac{1}{100}\sqrt{15}$	$\frac{31}{175}+\frac{1}{100}\sqrt{15}$	$\frac{128}{525}$	$\frac{31}{175}+\frac{1}{100}\sqrt{15}$	$\frac{31}{175}-\frac{1}{100}\sqrt{15}$	$\frac{1}{42}$

$\eta_1 = \left(495+66\sqrt{15}\right)^{1/2}$

$\eta_2 = \left(825+110\sqrt{15}\right)^{1/2}$

$\eta_3 = \left(495-66\sqrt{15}\right)^{1/2}$

$\eta_4 = \left(825-110\sqrt{15}\right)^{1/2}$

$[c_0, c_1, c_2, c_3, c_4, c_5, c_6] = [0,\ \frac{1}{2}-\frac{1}{66}\eta_1,\ \frac{1}{2}-\frac{1}{66}\eta_3,\ \frac{1}{2},\ \frac{1}{2}+\frac{1}{66}\eta_3,\ \frac{1}{2}+\frac{1}{66}\eta_1,\ 1]$