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# Block Boundary Value Methods for Linear Hamiltonian Systems

L. Brugnano and D. Trigiante

*Dipartimento di Energetica*
*Via C. Lombroso 6/17*
*50134 Firenze, Italy*

ABSTRACT

The problem of characterizing multistep methods suitable to efficiently approximate the solutions of linear Hamiltonian systems is discussed, showing that the appropriate methods should belong to the class of discrete Boundary Value Methods (BVMs). Three families of such methods are proposed. The presented methods have infinite regions of Absolute stability and can be of any order. In fact, for every odd $k$ there are $k$-step methods of order up to $2k$, which is the maximum order reachable by a $k$-step formula. © *Elsevier Science Inc., 1997*

## 1. INTRODUCTION

When finite arithmetic is used, appropriate methods based on discrete boundary value problems (BVPs) are able to control the growth of the errors much better than initial value methods (IVMs). The most famous example which supports this assertion is the so-called "Miller Algorithm" and its generalizations [1, 2]. Other examples can be found in standard books of Numerical Analysis [3, Example 1.3.4].

Boundary Value Methods (BVMs) are a class of methods for ODEs, based on linear multistep formulae, initially designed to take advantage of the above mentioned principle. Moreover, owing to their higher flexibility with respect to LMFs used as IVMs, they are able to reproduce the qualitative behavior of larger classes of continuous problems.

In this paper, we shall study the applicability of BVMs to linear Hamiltonian systems. The question has already been studied by Eirola and Sanz-Serna [4] for LMFs used with only initial conditions. They were able to give conditions on the coefficients of LMFs in order to maintain some important properties of continuous Hamiltonian problems. The pessimistic conclusion of the authors was that such conditions were not satisfied by methods with appropriate stability regions. It will be shown that this

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conclusion is no longer valid for BVMs, where there are a lot of methods (of any order and with infinite stability regions) satisfying the conditions given in [4].

The present approach, however, is different from the one used by the above-mentioned authors because we prefer to use a global one, which allows obtaining more general results.

In Sections 2 and 3, we shall briefly recall the main facts about linear Hamiltonian systems and BVMs, respectively. In Section 4, we discuss the application of BVMs to linear Hamiltonian problems. Finally, in Section 5, we describe three families of methods, and we present some numerical results.

## 2. HAMILTONIAN SYSTEMS

In this paper we shall restrict our analysis to linear Hamiltonian problems, that is, problems having the following form

$$\begin{aligned} y' &= Ly, \qquad t \in [t_0, T], \\ y(t_0) &= y_0 \in \mathbb{R}^{2m}, \end{aligned} \tag{1}$$

where, by denoting with $I_m$ the identity matrix of order $m$,

$$L = J_{2m}S, \qquad J_{2m} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes I_m, \qquad S = S^T.$$

The main features of the previous problem are

1. when $S$ is definite, the matrix $L$ is diagonalizable and has all purely imaginary eigenvalues;
2. for $h > 0$, $Q(hL) = e^{hJ_{2m}S}$ is a symplectic matrix, that is,

$$Q(hL)^T J_{2m} Q(hL) = J_{2m};$$

3. for every matrix $C$ such that $L^TC + CL = O$, the quadratic form

$$V(t; C) = y(t)^T C y(t)$$

is a constant of motion. In particular, for $C = S$, one obtains the Hamiltonian function of the problem.

One wishes to construct methods such that the previous Properties 2 and 3 are preserved. Such methods are usually called *symplectic methods*. So far, they have been essentially derived by looking for symplectic approximations to the matrix $Q(hL)$. Here, however, we shall follow a different approach. Before that, we need to recall the definition of BVMs.

## 3. BOUNDARY VALUE METHODS

Let a uniform mesh be defined on the integration interval $[t_0, T]$. The class of methods known as BVMs can be defined in different ways. The simplest one is to start with a $k$-step LMF and release the request to assign all the $k$ conditions required by the discrete problem at the initial points of the mesh. One takes the freedom to impose some of them, say $k_1 \geq 1$, at the initial points and the remaining $k_2 := k - k_1$ at the final ones. In other words, the continuous initial value problem (1) is approximated by means of a discrete boundary value problem with $(k_1, k_2)$*-boundary conditions*. The obtained discrete problems define the class of Boundary Value Methods. The usual concepts of stability (0-stability, Absolute stability, $A$-stability, etc.) are adequately generalized to such methods with the only difference that, this time, such concepts will depend on the couple $(k_1, k_2)$. One then speaks, for example, about $0_{k_1k_2}$-stability, $(k_1, k_2)$-Absolute stability regions, $A_{k_1k_2}$-stability, which reduce to the usual notions, when $k_1 = k$ and $k_2 = 0$ [5]. In this way, the flexibility and potentiality of LMFs dramatically increase. For example, by choosing the most appropriate couple $(k_1, k_2)$ of boundary conditions, one obtains $0_{k_1k_2}$-stable and $A_{k_1k_2}$-stable methods of arbitrary high order, including, for each odd value of $k$, the highest order $2k$.

An excellent example of the mentioned flexibility is the case of linear Hamiltonian problems. Suppose, for simplicity, that the matrix $S$ of problem (1) is definite, so that the eigenvalues of $L$ are purely imaginary. If one asks that, for all values of the stepsize $h$, the discrete solution has the same qualitative behavior of the continuous one, then one concludes that the boundary of the Absolute stability region must coincide with the imaginary axis. In this case, in fact, both the continuous and the discrete solutions are *marginally stable*.

It is well known that, apart from the trapezoidal rule, there are no LMFs which, when used with only initial conditions, have such property. The situation changes for BVMs. In Section 5 three families of such methods will be presented, all of them satisfying the above requirement.

The actual implementation of these methods proceeds by considering that a $k$-step linear multistep formula applied to problem (1) gives the discrete equation

$$\sum_{i=0}^{k}(\alpha_i I_{2m} - h\beta_i L)y_{n+i} = 0. \tag{2}$$

If the partition $t_0 < t_1 < \cdots < t_{N+k_2-1} \equiv T$ is considered, then the unknowns are

$$y_0, y_1, \ldots, y_{N+k_2-1},$$

while (2) can be used only for $n = 0, \ldots, N-k_1-1$, thus providing $N-k_1$ equations. The continuous problem provides the initial value $y_0$, thus reducing the number of the unknowns to $N+k_2-1$. Suppose that the given formula has to be used with $(k_1, k_2)$-boundary conditions. Instead of providing the $k_1 - 1$ additional initial values, we introduce $k_1 - 1$ additional initial equations (of course independent of (2)). These are obtained by using a set of suitable methods (*additional initial methods*). Similarly, instead of fixing the $k_2$ final additional values, we introduce $k_2$ additional final equations (*additional final methods*). Suppose that all the additional methods have $r$ steps. Then we have the following set of equations.

$$\begin{array}{rl}
y_0 \quad \text{given} & \}\ \text{continuous problem,} \\
\left.\begin{array}{r} I_1(y_0, \ldots, y_r) = 0 \\ \vdots \\ I_{k_1-1}(y_0, \ldots, y_r) = 0 \end{array}\right\} & \text{additional initial methods,} \\
\left.\begin{array}{r} M_1(y_0, \ldots, y_k) = 0 \\ \vdots \\ M_{N-k_1}(y_{N-k_1}, \ldots, y_{N+k_2-1}) = 0 \end{array}\right\} & \text{main method,} \\
\left.\begin{array}{r} F_1(y_{N+k_2-1-r}, \ldots, y_{N+k_2-1}) = 0 \\ \vdots \\ F_{k_2}(y_{N+k_2-1-r}, \ldots, y_{N+k_2-1}) = 0 \end{array}\right\} & \text{additional final methods.}
\end{array}$$

One then obtains a set of $N + k_2$ equations in the same number of unknowns. The overall process can be considered as a composite initial value method. Moreover, if one replaces the initial value $y_0$ with a more general condition

$$P(y_0, y_1, \ldots, y_{N+k_2-1}) = 0,$$

the same procedure can also be used for solving continuous BVPs [6].

Written in this way, a BVM no longer requires the final additional values, thus removing one of the main objection against these methods. Moreover, to a certain extent, a BVM may also be regarded as a generalization of a Runge-Kutta scheme, by assimilating the additional relations (both initial and final) to the stages of a Runge-Kutta method.

## 4. APPLICATION OF BVMs TO LINEAR HAMILTONIAN SYSTEMS

We now consider the application of BVMs to problem (1), by recasting the discrete problem in matrix form. Let us define the matrices

$$
\begin{aligned}
A &= \begin{pmatrix} \alpha_0 & \alpha_1 & \cdots & \alpha_k & & & & \\ & \ddots & \ddots & & \ddots & & O & \\ & & \ddots & \ddots & & \ddots & & \\ & O & & \ddots & \ddots & & \ddots & \\ & & & & \alpha_0 & \alpha_1 & \cdots & \alpha_k \end{pmatrix}_{(N-k_1)\times(N+k_2)}, \\
B &= \begin{pmatrix} \beta_0 & \beta_1 & \cdots & \beta_k & & & & \\ & \ddots & \ddots & & \ddots & & O & \\ & & \ddots & \ddots & & \ddots & & \\ & O & & \ddots & \ddots & & \ddots & \\ & & & & \beta_0 & \beta_1 & \cdots & \beta_k \end{pmatrix}_{(N-k_1)\times(N+k_2)},
\end{aligned} \tag{3}
$$

made up with the coefficients of the main method. Then, we define the following augmented matrices

$$
\begin{aligned}
\widetilde{A} &= \begin{pmatrix} (A_I \quad O) \\ A \\ (O \quad A_F) \end{pmatrix}_{(N+k_2-1)\times(N+k_2)}, \\
\widetilde{B} &= \begin{pmatrix} (B_I \quad O) \\ B \\ (O \quad B_F) \end{pmatrix}_{(N+k_2-1)\times(N+k_2)},
\end{aligned} \tag{4}
$$

where

$$A_I = \begin{pmatrix} \alpha_0^{(1)} & \dots & \alpha_r^{(1)} \\ \vdots & & \vdots \\ \alpha_0^{(k_1-1)} & \dots & \alpha_r^{(k_1-1)} \end{pmatrix}, \quad B_I = \begin{pmatrix} \beta_0^{(1)} & \dots & \beta_r^{(1)} \\ \vdots & & \vdots \\ \beta_0^{(k_1-1)} & \dots & \beta_r^{(k_1-1)} \end{pmatrix},$$

$$A_F = \begin{pmatrix} \alpha_0^{(N)} & \dots & \alpha_r^{(N)} \\ \vdots & & \vdots \\ \alpha_0^{(N+k_2-1)} & \dots & \alpha_r^{(N+k_2-1)} \end{pmatrix}, \tag{5}$$

$$B_F = \begin{pmatrix} \beta_0^{(N)} & \dots & \beta_r^{(N)} \\ \vdots & & \vdots \\ \beta_0^{(N+k_2-1)} & \dots & \beta_r^{(N+k_2-1)} \end{pmatrix},$$

and $\alpha_i^{(j)}$, $\beta_i^{(j)}$, $i = 0,1,\dots,r$, are the coefficients of the initial ($j = 1,\dots,k_1-1$) and final ($j = N, N+1,\dots,N+k_2-1$) additional methods. Finally, let

$$\mathbf{y} = (y_0,\dots,y_{N+k_2-1})^T \tag{6}$$

be the block vector which contains the discrete solution. Then, it is not difficult to see that this vector satisfies the equation

$$M\mathbf{y} := (\widetilde{A} \otimes I_{2m} - h\widetilde{B} \otimes J_{2m}S)\mathbf{y} = \mathbf{0}. \tag{7}$$

This means that $\mathbf{y}$ belongs to the null space of $M$, which has dimension $1 \cdot (2m)$, thus reflecting the fact that there is only one more condition to be imposed, which, of course, is the one provided by the initial condition $y_0$. In this case, in fact, the discrete solution (6) is obtained by solving the linear system

$$\widehat{M}\mathbf{y} := \begin{pmatrix} (I_{2m} \quad O) \\ M \end{pmatrix} \mathbf{y} = \begin{pmatrix} y_0 \\ \mathbf{0} \end{pmatrix}. \tag{8}$$

Therefore, in the following we assume the matrix $\widehat{M}$ to be nonsingular.

In order to choose the most appropriate main and additional methods for problem (1), suppose changing the independent variable by posing $\tau = t_0 + t_{N+k_2-1} - t$, where $t_{N+k_2-1} \equiv T$ is the end of the integration interval. This changes problem (1) into

$$\frac{dy}{d\tau} = -J_{2m}Sy, \tag{9}$$

and reverses the interval of integration; Equation (9) is still Hamiltonian and then the same numerical method would be appropriate to it. This is nothing but the *time isotropy* (or *time reversal symmetry*) of Hamiltonian systems. We shall use this property for choosing the numerical methods. In fact, by reversing the boundary conditions, they should provide the same discrete solution in the reverse order. Thus, let us define the permutation matrix

$$P_s = \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & \cdot & & \\ & \cdot & & & \\ 1 & & & & \end{pmatrix}_{s \times s} \tag{10}$$

and the vector

$$\mathbf{z} = (P_{N+k_2} \otimes I_{2m})\mathbf{y} \equiv (y_{N+k_2-1}, \ldots, y_1, y_0)^T.$$

At this point, we require that

$$P_{N+k_2-1}\widetilde{A}P_{N+k_2} = -\widetilde{A}, \qquad P_{N+k_2-1}\widetilde{B}P_{N+k_2} = \widetilde{B}. \tag{11}$$

Then, multiplication on the left of Equation (7) by $P_{N+k_2-1} \otimes I_{2m}$ gives

$$\begin{aligned} \mathbf{0} &= (P_{N+k_2-1} \otimes I_{2m})(\widetilde{A} \otimes I_{2m} - h\widetilde{B} \otimes J_{2m}S)\mathbf{y} \\ &= (P_{N+k_2-1}\widetilde{A}P_{N+k_2} \otimes I_{2m} - hP_{N+k_2-1}\widetilde{B}P_{N+k_2} \otimes J_{2m}S) \\ &\quad \times (P_{N+k_2} \otimes I_{2m})\mathbf{y} \\ &= -(\widetilde{A} \otimes I_{2m} - h\widetilde{B} \otimes (-J_{2m}S))\mathbf{z}, \end{aligned}$$

that is, the vector $\mathbf{z}$ is obtainable by direct application of the method to problem (9). We observe that the requirement

$$P_{N+k_2-1}\widetilde{A}P_{N+k_2} = \widetilde{A}, \qquad P_{N+k_2-1}\widetilde{B}P_{N+k_2} = -\widetilde{B},$$

would produce the same effect. However, it is not compatible with the consistency conditions for the methods.

Let us examine in more details the requirement (11). First of all, from (4) and (5), it follows that

$$k_1 - 1 = k_2 \equiv \nu, \tag{12}$$

that is, the number of steps $k = k_1 + k_2 \equiv 2\nu + 1$ of the main method must be odd. Moreover, it is easy to verify that the coefficients of the main method must satisfy the following relation

$$\alpha_i = -\alpha_{k-i}, \quad \beta_i = \beta_{k-i}, \qquad i = 0, 1, \ldots, k. \tag{13}$$

Similarly, for the coefficients of the additional methods, one must have

$$\alpha_i^{(j)} = -\alpha_{r-i}^{(N+\nu-j)}, \quad \beta_i^{(j)} = \beta_{r-i}^{(N+\nu-j)}, \quad i = 0, \ldots, r, \quad j = 1, \ldots, \nu. \tag{14}$$

We shall call *symmetric schemes* the BVMs which satisfy (11) and, therefore, (12)–(14). We observe that the popular mid-point method,

$$y_{n+2} - y_n = 2hf_{n+1},$$

does not fit in this class, either when used as IVM or as BVM [7]. In fact, in the former case, one has $k_1 - 1 = 1$, $k_2 = 0$, and $k_1 - 1 = 0$ and $k_2 = 1$ in the latter one.

The symmetry conditions (11) are important, not only because they permit the efficient design of the methods, but also because they allow the derivation of the conservation laws for the discrete system, as we are going to see. Before that, we need to state some preliminary results and notations.

Let $Q_0$ and $Q_1$ be the permutation matrices of dimension $(N+\nu)^2$ and $(N+\nu-1)^2$ such that

$$Q_i \begin{pmatrix} 1 \\ 2 \\ \vdots \\ (N+\nu-i)^2 \end{pmatrix} = \begin{pmatrix} 1 \\ (N+\nu-i)+1 \\ 2(N+\nu-i)+1 \\ \vdots \\ 2 \\ (N+\nu-i)+2 \\ \vdots \\ (N+\nu-i) \\ \vdots \\ (N+\nu-i)^2 \end{pmatrix}, \qquad i = 0, 1.$$

Furthermore, by considering the partitioning,

$$\widetilde{A} = (\widetilde{A}_1 \; a_2), \qquad \widetilde{B} = (\widetilde{B}_1 \; b_2), \qquad a_2, b_2 \in \mathbb{R}^{N+\nu-1}, \tag{15}$$

we define

$$R = \widetilde{A}_1^T \otimes \widetilde{B}_1^T + \widetilde{B}_1^T \otimes \widetilde{A}_1^T. \tag{16}$$

Consider now the following system of linear equations

$$(\widetilde{A}^T \otimes \widetilde{B}^T + \widetilde{B}^T \otimes \widetilde{A}^T)\mathbf{g} = \mathbf{h}, \tag{17}$$

where the unknown vector $\mathbf{g} \in \mathbb{R}^{(N+\nu-1)^2}$, and $\mathbf{h} \in \mathbb{R}^{(N+\nu)^2}$ is such that

$$(P_{N+\nu} \otimes P_{N+\nu})\mathbf{h} = -\mathbf{h}, \qquad Q_0\mathbf{h} = \mathbf{h}. \tag{18}$$

Then, the following result holds true.

LEMMA 4.1. *Suppose that*

i) *the condition* (11) (*i.e.,* (13) *and* (14)) *is satisfied;*
ii) *the square matrix* $R$ *defined in* (16) *is nonsingular.*

*Then, there exists a unique solution vector* $\mathbf{g}$ *of* (17)–(18), *which also satisfies the relations*

$$(P_{N+\nu-1} \otimes P_{N+\nu-1})\mathbf{g} = \mathbf{g}, \qquad Q_1\mathbf{g} = \mathbf{g}. \tag{19}$$

PROOF. By partitioning the two matrices $\widetilde{A}$ and $\widetilde{B}$ as in (15), it follows that the coefficient matrix of Equation (17) has full column rank. In fact, one has

$$\begin{aligned}\widetilde{A}^T \otimes \widetilde{B}^T + \widetilde{B}^T \otimes \widetilde{A}^T &= \begin{pmatrix} \widetilde{A}_1^T \\ a_2^T \end{pmatrix} \otimes \begin{pmatrix} \widetilde{B}_1^T \\ b_2^T \end{pmatrix} + \begin{pmatrix} \widetilde{B}_1^T \\ b_2^T \end{pmatrix} \otimes \begin{pmatrix} \widetilde{A}_1^T \\ a_2^T \end{pmatrix} \\ &= \begin{pmatrix} \widetilde{A}_1^T \otimes \begin{pmatrix} \widetilde{B}_1^T \\ b_2^T \end{pmatrix} + \widetilde{B}_1^T \otimes \begin{pmatrix} \widetilde{A}_1^T \\ a_2^T \end{pmatrix} \\ a_2^T \otimes \begin{pmatrix} \widetilde{B}_1^T \\ b_2^T \end{pmatrix} + b_2^T \otimes \begin{pmatrix} \widetilde{A}_1^T \\ a_2^T \end{pmatrix} \end{pmatrix}. \end{aligned} \tag{20}$$

Then, from hypothesis ii), the equations corresponding to the matrix $R$ are independent. We shall prove later that the remaining equations are redundant, so that there exists a unique solution vector $\mathbf{g}$ of problem (17)–(18). Before that, we show that if a solution exists, it will satisfy (19). In fact, from (11)–(12), one has that

$$\begin{aligned} -\mathbf{h} &= (P_{N+\nu} \otimes P_{N+\nu})\mathbf{h} \\ &= (P_{N+\nu} \otimes P_{N+\nu})(\widetilde{A}^T \otimes \widetilde{B}^T + \widetilde{B}^T \otimes \widetilde{A}^T)\mathbf{g} \\ &= -(\widetilde{A}^T \otimes \widetilde{B}^T + \widetilde{B}^T \otimes \widetilde{A}^T)(P_{N+\nu-1} \otimes P_{N+\nu-1})\mathbf{g}; \end{aligned}$$

that is, $\mathbf{g}$ is a solution of (17) iff $(P_{N+\nu-1} \otimes P_{N+\nu-1})\mathbf{g}$ is also a solution. The first equality in (19) then follows from the fact that the coefficient matrix (20) has full column rank. Similarly, the second equality follows by considering that

$$\begin{aligned}\mathbf{h} &= Q_0\mathbf{h}\\ &= Q_0(\widetilde{A}^T \otimes \widetilde{B}^T + \widetilde{B}^T \otimes \widetilde{A}^T)Q_1Q_1\mathbf{g}\\ &= (\widetilde{B}^T \otimes \widetilde{A}^T + \widetilde{A}^T \otimes \widetilde{B}^T)Q_1\mathbf{g}.\end{aligned}$$

Finally, let us show that the equations in (17) not corresponding to the matrix $R$ are redundant. For brevity, we shall only prove the redundancy of the last equation in (17), because similar arguments can be used for the remaining ones. Let us denote by $a_1^T$ and $b_1^T$ the first rows of the matrices $\widetilde{A}_1^T$ and $\widetilde{B}_1^T$, respectively. From (11), it follows that

$$a_2^T = -a_1^T P_{N+\nu-1}, \qquad b_2^T = b_1^T P_{N+\nu-1}.$$

As a consequence, if $\mathbf{e}_i$ is the $i$th vector of the canonical base in $\mathbb{R}^{N+\nu}$, one has

$$\begin{aligned}(a_2^T \otimes b_2^T + b_2^T \otimes a_2^T)\mathbf{g} &= (\mathbf{e}_{N+\nu}^T \otimes \mathbf{e}_{N+\nu}^T)(\widetilde{B}^T \otimes \widetilde{A}^T + \widetilde{A}^T \otimes \widetilde{B}^T)\mathbf{g}\\ &= (\mathbf{e}_{N+\nu}^T \otimes \mathbf{e}_{N+\nu}^T)\mathbf{h}\\ &= -(\mathbf{e}_1^T \otimes \mathbf{e}_1^T)\mathbf{h},\end{aligned} \tag{21}$$

where the last equality follows from (18). The thesis is then completed by observing that from (19),

$$\begin{aligned}(a_2^T \otimes b_2^T + b_2^T \otimes a_2^T)\mathbf{g} &= (a_2^T \otimes b_2^T + b_2^T \otimes a_2^T)(P_{N+\nu-1} \otimes P_{N+\nu-1})\mathbf{g}\\ &= -(a_1^T \otimes b_1^T + b_1^T \otimes a_1^T)\mathbf{g},\end{aligned}$$

which shows that the first and the last equation in (17) are equivalent. ∎

We are in the position to state the following main result.

THEOREM 4.1. *Suppose that*

i) *the hypotheses of Lemma* 4.1 *are satisfied;*
ii) *$C$ is a matrix such that* $CL + L^TC = O$.

*Then, if* $\mathbf{y}$ *is any solution of system* (7), *for all* $i, j = 0, \dots, N+\nu-1$, *one has,*

$$y_i^T C y_j + y_j^T C y_i = y_{N+\nu-1-i}^T C y_{N+\nu-1-j} + y_{N+\nu-1-j}^T C y_{N+\nu-1-i}. \tag{22}$$

PROOF. Let $G$ be any symmetric matrix of dimension $N+\nu-1$, such that

$$P_{N+\nu-1} G P_{N+\nu-1} = G,$$

that is, $G$ is also centrosymmetric. Multiplication on the left of (7) by $\mathbf{y}^T(\widetilde{B}^T G \otimes C)$ gives

$$\mathbf{y}^T(\widetilde{B}^T G\widetilde{A} \otimes C - h\widetilde{B}^T G\widetilde{B} \otimes CL)\mathbf{y} = 0.$$

Similarly, multiplication on the left by $\mathbf{y}^T(\widetilde{B}^T G \otimes C^T)$ gives

$$\mathbf{y}^T(\widetilde{B}^T G\widetilde{A} \otimes C^T - h\widetilde{B}^T G\widetilde{B} \otimes C^T L)\mathbf{y} = 0.$$

By adding the transpose of the latter expression to the former one, from the hypothesis ii) it follows that

$$\begin{aligned} 0 &= \mathbf{y}^T((\widetilde{B}^T G\widetilde{A} + \widetilde{A}^T G\widetilde{B}) \otimes C - h\widetilde{B}^T G\widetilde{B} \otimes (CL + L^T C))\mathbf{y} \\ &= \mathbf{y}^T((\widetilde{B}^T G\widetilde{A} + \widetilde{A}^T G\widetilde{B}) \otimes C)\mathbf{y} \\ &\equiv \mathbf{y}^T(H_G \otimes C)\mathbf{y}. \end{aligned} \tag{23}$$

From (11), the symmetric matrix

$$H_G = \widetilde{B}^T G\widetilde{A} + \widetilde{A}^T G\widetilde{B} \tag{24}$$

is such that

$$\begin{aligned} P_{N+\nu} H_G P_{N+\nu} &= P_{N+\nu}\widetilde{B}^T P_{N+\nu-1} P_{N+\nu-1} G P_{N+\nu-1} P_{N+\nu-1}\widetilde{A} P_{N+\nu} \\ &\quad + P_{N+\nu}\widetilde{A}^T P_{N+\nu-1} P_{N+\nu-1} G P_{N+\nu-1} P_{N+\nu-1}\widetilde{B} P_{N+\nu} \\ &= -\widetilde{B}^T G\widetilde{A} - \widetilde{A}^T G\widetilde{B} \\ &= -H_G. \end{aligned}$$

Then, by writing such matrix as

$$H_G = \begin{pmatrix} 2h_{00} & h_{01} & \cdots & h_{0,N+\nu-1} \\ h_{10} & 2h_{11} & \ddots & \vdots \\ \vdots & \ddots & \ddots & h_{N+\nu-2,N+\nu-1} \\ h_{N+\nu-1,0} & \cdots & h_{N+\nu-1,N+\nu-2} & 2h_{N+\nu-1,N+\nu-1} \end{pmatrix},$$

it follows that for all $i, j = 0, \dots, N+\nu-1$,

$$h_{ij} = h_{ji} = -h_{N+\nu-1-i,N+\nu-1-j} = -h_{N+\nu-1-j,N+\nu-1-i}. \tag{25}$$

As a consequence, (23) reduces to

$$\sum_{i=0}^{N+\nu-1} \sum_{j=i}^{N+\nu-1-i} h_{ij}\xi_{ij} = 0, \tag{26}$$

where

$$\xi_{ij} = y_i^T C y_j + y_j^T C y_i - y_{N+\nu-1-i}^T C y_{N+\nu-1-j} - y_{N+\nu-1-j}^T C y_{N+\nu-1-i}.$$

It remains to be seen that (26) implies that $\xi_{ij} = 0$ for all values of $i$ and $j$. This follows from the fact that the matrix $H_G$ satisfying (25) can be chosen arbitrarily, so that (26) must hold true for every choice of the scalars $\{h_{ij}\}$. To prove this part, we remember that, given an $m \times n$ matrix $X$, vec($X$) is the $mn$ vector made up with the entries of its columns [8]

$$\mathrm{vec}(X) = \begin{pmatrix} X_{*1} \\ X_{*2} \\ \vdots \\ X_{*n} \end{pmatrix}.$$

By posing

$$\mathbf{g} = \mathrm{vec}(G), \qquad \mathbf{h} = \mathrm{vec}(H_G),$$

one has that (24) can be posed in the tensor form (17). Moreover, due to (25), the vector **h** satisfies (18). Because the hypotheses of Lemma 4.1 are fulfilled, it follows that for every vector **h** satisfying (18) there exists a vector **g** satisfying (17) and (19). This means that every matrix $H_G$ satisfying (25) can be obtained from (24), by using a suitable symmetric and centrosymmetric matrix $G$. ■

The discrete conservation property corresponding to Property 3 seen in Section 2, can now be easily derived, as shown by the next corollary.

COROLLARY 4.1. *The constants of motion of problem* (1) *are exactly preserved in the last point of the discrete solution.*

PROOF. Let $C$ be any matrix such that $CL + L^T C = O$. The result of Theorem 4.1 then applies, so that for $i = j = 0$, from (22), one obtains

$$y_0^T C y_0 = y_{N+\nu-1}^T C y_{N+\nu-1}.$$ ■

REMARK 4.1. When $C = S$, one obtains the conservation for the Hamiltonian function. Moreover, from (22) and $j = i$, one obtains that

$$y_i^T C y_i = y_{N+\nu-1-i}^T C y_{N+\nu-1-i}, \qquad i = 0, \dots, N+\nu-1, \tag{27}$$

that is, the approximations of the constants of motion assume symmetric values in the interval of integration $[t_0, T]$.

In Property 2 reported in Section 2, it was remarked that for each $h$, the map $Q(hL)$ is symplectic for the continuous flow. A similar result holds for the discrete map associated with the method described by Equation (8). In fact, by considering the block vector

$$\mathbf{\Phi} = \widehat{M}^{-1} \begin{pmatrix} I_{2m} \\ O \end{pmatrix} \equiv \begin{pmatrix} \phi_0 \\ \vdots \\ \phi_{N+\nu-1} \end{pmatrix}, \quad \phi_i \in \mathbb{R}^{2m\times 2m}, \quad i = 0, \dots, N+\nu-1,$$

one easily verifies that its $i$th block entry defines the map $y_i = \phi_i y_0$. Moreover, the block vector $\mathbf{\Phi}$ satisfies Equation (7), so that from Theorem 4.1, by taking $C = J_{2m}$, one obtains that, for all $i, j = 0, \dots, N+\nu-1$,

$$\begin{aligned} \phi_i^T J_{2m} \phi_j + \phi_j^T J_{2m} \phi_i = \phi_{N+\nu-1-i}^T J_{2m} \phi_{N+\nu-1-j} \\ + \phi_{N+\nu-1-j}^T J_{2m} \phi_{N+\nu-1-i}. \end{aligned} \tag{28}$$

As a consequence, we obtain the discrete analog of Property 2 seen in Section 2.

COROLLARY 4.2. *The map* $y_{N+\nu-1} = \phi_{N+\nu-1} y_0$ *is symplectic.*

PROOF. By recalling that $\phi_0 = I_{2m}$, for $i = j = 0$ (28) gives

$$\phi_{N+\nu-1}^T J_{2m} \phi_{N+\nu-1} = J_{2m}. \qquad \blacksquare$$

In addition to the previous result, it is possible to show that if the method has order $p$, then for $i = 1, \dots, N+\nu-2$

$$\phi_i = Z^i + O(h^p \gamma^{\min(i, N+\nu-1-i)}),$$

where $Z$ is a symplectic matrix and $0 < \gamma < 1$ [9].

## 5. BLOCK SYMMETRIC SCHEMES

We now present three families of symmetric schemes. All of them can be regarded as generalizations of the basic trapezoidal rule. In fact, the boundary of the corresponding $(\nu+1,\nu)$-Absolute stability regions (see (12)) coincides with the imaginary axis, and, for each family, the simplest formula, obtained for $\nu = 0$, is the trapezoidal rule. Moreover, all these methods satisfy the hypotheses of Lemma 4.1.

It has been proved in the last section that symmetric BVMs (i.e., satisfying (11)) preserve the constants of motion of the continuous problem at the points $t_0$ and $t_\mu$, where, for brevity, $\mu$ denotes the index of the last point of the block. To take advantage of this fact, we divide the interval of integration $[t_0, T]$ in a certain number $\ell$ of subintervals:

$$[t_0, t_\mu],\ [t_\mu, t_{2\mu}], \dots, [t_{(\ell-1)\mu}, T].$$

Then we apply the same symmetric scheme on each of these subintervals, so that the final point of each block will be the initial one for the subsequent. This permits having the exact values of the constants of motion at $t_0, t_\mu, \dots, t_{(\ell-1)\mu}, T$.

This approach, which turns out to be more appropriate for linear Hamiltonian systems, allows a very efficient parallel implementation of these methods [10]. Concerning the order of the additional methods, we take them of the same order of the main method, even if, in general, they can be taken one order smaller [6, 9].

In the following, $k = 2\nu + 1$ is the number of steps of the schemes.

### *5.1. Extended trapezoidal rules*

The Extended Trapezoidal Rules (ETRs) [11] have the following form

$$y_n - y_{n-1} = h \sum_{i=0}^{\nu} \beta_i (f_{n-\nu-1+i} + f_{n+\nu-i}), \qquad n = \nu+1, \dots, N-1.$$

The coefficients $\{\beta_i\}$ are determined by imposing that the method has the highest possible order, that is, $p = k+1 \equiv 2(\nu+1)$. The additional equations are given by

$$\left.\begin{aligned} y_r - y_{r-1} &= h \sum_{i=0}^{k} \beta_{i,r} f_i, \\ y_{N+\nu-r} - y_{N+\nu-r-1} &= h \sum_{i=0}^{k} \beta_{i,r} f_{N+\nu-1-i}, \end{aligned}\right. \qquad r = 1, \dots, \nu,$$

where the coefficients $\{\beta_{i,r}\}$ are determined by imposing that the corresponding formula has order $k+1$. These coefficients obviously satisfy (14).

EXAMPLE 5.1. For $\nu = 1$, we get the fourth order ETR

$$y_n - y_{n-1} = \frac{h}{24}(-f_{n+1} + 13f_n + 13f_{n-1} - f_{n-2}), \qquad n = 2, \ldots, N-1.$$

It can be conveniently used with the following two additional equations

$$y_1 - y_0 = \frac{h}{24}(f_3 - 5f_2 + 19f_1 + 9f_0),$$

and

$$y_N - y_{N-1} = \frac{h}{24}(9f_N + 19f_{N-1} - 5f_{N-2} + f_{N-3}).$$

*5.2. Extended trapezoidal rules of second kind*

ETRs can be regarded as generalizations of the basic trapezoidal rule which preserve the structure of the first characteristic polynomial $\rho(z)$. Similarly, we may obtain another family of methods which preserve the structure of the second characteristic polynomial, $\sigma(z)$, of the same basic scheme. The following methods, which we call Extended Trapezoidal Rules of second kind ($\mathrm{ETR_2}$s), are then obtained [9, 12]

$$\sum_{i=0}^{\nu} \alpha_i (y_{n-\nu-1+i} - y_{n+\nu-i}) = \frac{h}{2}(f_n + f_{n-1}), \qquad n = \nu+1, \ldots, N-1.$$

As in the case of ETRs, the coefficients $\{\alpha_i\}$ are determined by imposing that the considered formula has the highest possible order, that is, $p = k+1 \equiv 2(\nu+1)$. The following additional equations can be used for the additional conditions

$$\begin{aligned} \sum_{i=0}^{k} \alpha_{i,r} y_i &= h(\beta_r f_r + (1-\beta_r) f_{r-1}), \\ & \qquad\qquad\qquad\qquad r = 1, \ldots, \nu, \\ \sum_{i=0}^{k} -\alpha_{i,r} y_{N+\nu-1-i} &= h(\beta_r f_{N+\nu-1-r} + (1-\beta_r) f_{N+\nu-r}), \end{aligned}$$

where the coefficients $\{\alpha_{i,r}\}$ are determined by imposing the corresponding formula to have order $k+1$.

EXAMPLE 5.2. For $\nu = 1$, we obtain the following fourth order $\mathrm{ETR_2}$

$$\frac{1}{12}(y_{n+1} + 9y_n - 9y_{n-1} - y_{n-2}) = \frac{h}{2}(f_n + f_{n-1}), \qquad n = 2, \ldots, N-1.$$

In this case, the two required additional equations are given by

$$\frac{1}{24}(-y_3 + 9y_2 + 9y_1 - 17y_0) = \frac{h}{4}(3f_1 + f_0),$$
$$\frac{1}{24}(17y_N - 9y_{N-1} - 9y_{N-2} + y_{N-3}) = \frac{h}{4}(f_N + 3f_{N-1},).$$

*5.3. Top order methods*

The last family of methods we consider is that of Top Order Methods (TOMs). The name of these methods [12, 13] derives from the fact that the coefficients of the generic $k$-step ($k = 2\nu + 1$) method

$$\sum_{i=0}^{\nu} \alpha_i (y_{n-\nu-1+i} - y_{n+\nu-i})$$
$$= h \sum_{i=0}^{\nu} \beta_i (f_{n-\nu-1+i} + f_{n+\nu-i}), \quad n = \nu+1, \dots, N-1,$$

are determined so that the order $p = 2k \equiv 4\nu + 2$ is obtained, which is the maximum order reachable by a $k$-step LMF.

Appropriate additional equations for these formulae can be chosen, for example, as follows

$$\left.\begin{aligned} y_r - y_{r-1} &= h \sum_{i=0}^{2k-1} \beta_{i,r} f_i, \\ y_{N+\nu-r} - y_{N+\nu-r-1} &= h \sum_{i=0}^{2k-1} \beta_{i,r} f_{N+\nu-1-i}, \end{aligned}\right. \qquad r = 1, \dots, \nu,$$

where the coefficients $\{\beta_{i,r}\}$ are determined so that each formula has order $2k$.

EXAMPLE 5.3. For $\nu = 1$, we obtain the sixth-order TOM

$$\frac{1}{60}(11y_{n+1} + 27y_n - 27y_{n-1} - 11y_{n-2}) = \frac{h}{20}(f_{n+1} + 9f_n + 9f_{n-1} + f_{n-2}),$$

which can be used with the following two additional equations,

$$y_1 - y_0 = \frac{h}{1440}(27f_5 - 173f_4 + 482f_3 - 798f_2 + 1427f_1 + 475f_0),$$

and

$$y_N - y_{N-1} = \frac{h}{1440}(475 f_N + 1427 f_{N-1} - 798 f_{N-2} + 482 f_{N-3} - 173 f_{N-4} + 27 f_{N-5}).$$

We conclude this section with a simple numerical example, carried out by using the fourth-order ETR described in Example 5.1.

Consider the equation of the harmonic oscillator

$$y' = \begin{pmatrix} 0 & 1 \\ -9 & 0 \end{pmatrix} y, \qquad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad t \in [0, 50]. \tag{29}$$

The Hamiltonian function of problem (29) is

$$V(t) = 9y_1(t)^2 + y_2(t)^2.$$

In Figure 1, we report the obtained discrete solution with the fourth order ETR, used with five blocks and stepsize $h = 1$, and the corresponding

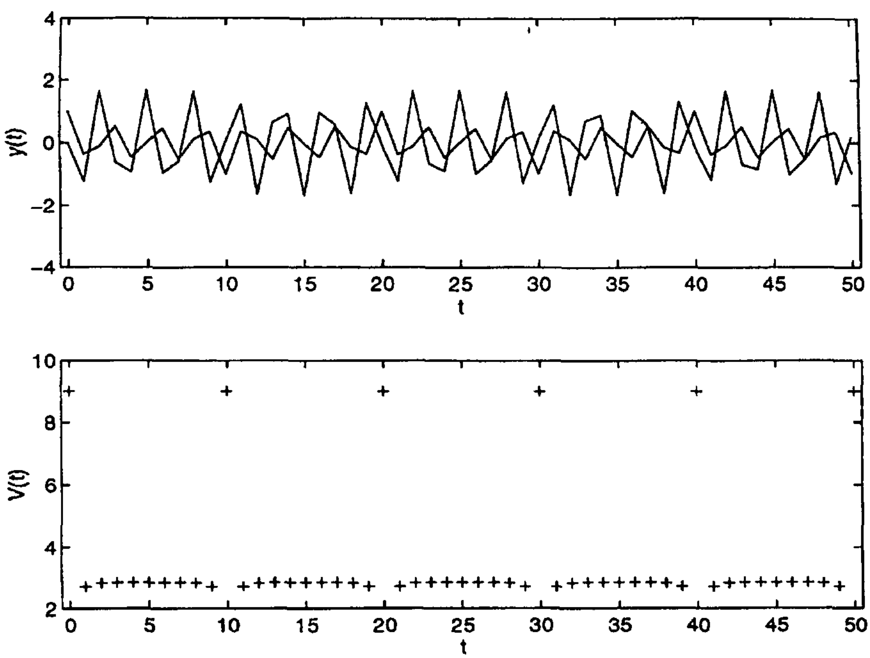


FIG. 1. Discrete solution for problem (29) and values of the Hamiltonian function (30) for the computed solution, $h = 1$.

values of

$$V_n = 9y_{1,n}^2 + y_{2,n}^2 \tag{30}$$

for the computed discrete solution. The predicted symmetry (27) inside each block is evident, as well as that the value $V_0$ is exactly maintained at the points $t = 0, 10, \dots, 50$, even if the obtained discrete solution provides a very poor approximation of the continuous one because of the large value of the stepsize used.

In Figure 2, we report the results on the same problem, but when a stepsize $h = 0.25$ is used. Again, the fourth order ETR has been used with five blocks. Now the solution is much better with respect to the previous case. This is reflected in the fact that all the values of the Hamiltonian function are much closer to the expected value $V = 9$, which is exactly preserved at the points $t = 0, 10, \dots, 50$. Also, in this case, the predicted symmetry (27) inside each block is evident. Finally, in Figure 3, we report the results obtained with stepsize $h = 0.125$.

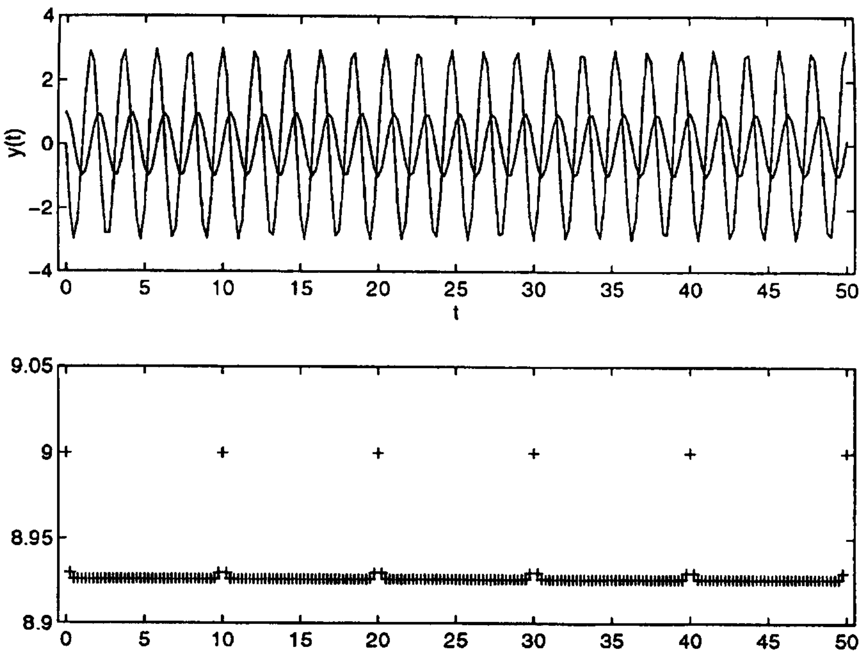


FIG. 2. Discrete solution for problem (29) and values of the Hamiltonian function (30) for the computed solution, $h = 0.25$.

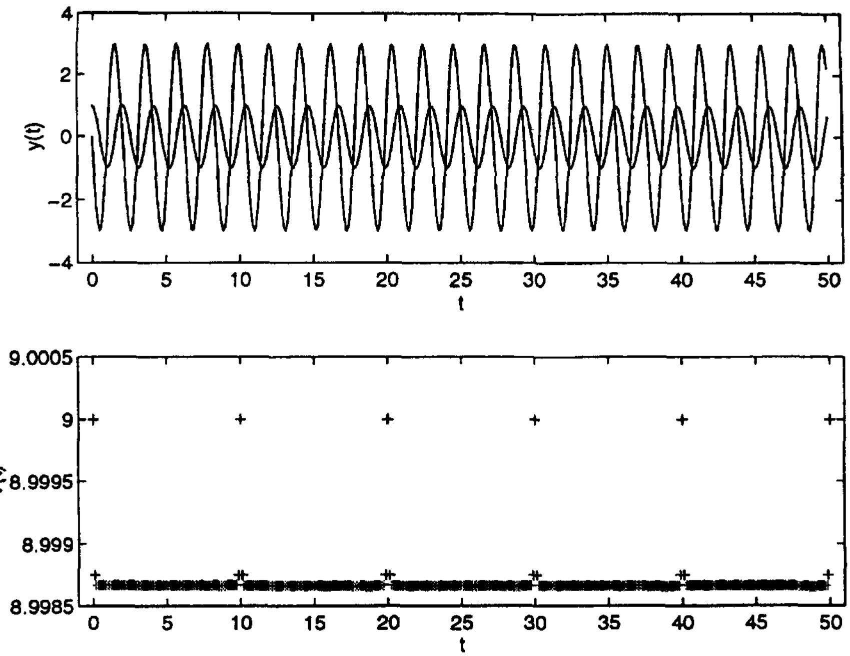


FIG. 3. Discrete solution for problem (29) and values of the Hamiltonian function (30) for the computed solution, $h = 0.125$.

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