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ESSENTIALLY SYMPLECTIC BOUNDARY VALUE METHODS FOR LINEAR HAMILTONIAN SYSTEMS*[1)]

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Abstract

In this paper we are concerned with finite difference schemes for the numerical approximation of linear Hamiltonian systems of ODEs. Numerical methods which preserves the qualitative properties of Hamiltonian flows are called *symplectic integrators*. Several symplectic methods are known in the class of Runge-Kutta methods. However, no high order symplectic integrators are known in the class of Linear Multistep Methods (LMMs). Here, by using LMMs as Boundary Value Methods (BVMs), we show that symplectic integrators of arbitrary high order are also available in this class. Moreover, these methods can be used to solve both initial and boundary value problems. In both cases, the properties of the flow of Hamiltonian systems are "essentially" maintained by the discrete map, at least for linear problems.

1. Introduction

In many areas of physics, mechanics, etc., Hamiltonian systems of ODEs play a very important role. Such systems have the following general form:

$$y' = J_{2m}^T \bigtriangledown H(y,t), \quad t \in [t_0, T], \quad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

where, by denoting with O_m and I_m the null matrix and the identity matrix of order m, respectively,

$$J_{2m} = \begin{pmatrix} O_m & I_m \\ -I_m & O_m \end{pmatrix}.$$

Simple properties of the matrix J_{2m} are the following ones:

$$J_{2m}^{-1} = J_{2m}^T = -J_{2m}, \qquad \det(J_{2m}) = 1.$$

In equation (1) $\bigtriangledown H(y,t)$ is the gradient of a scalar function $H(y,t)$, usually called *Hamiltonian*. In the case where $H(y,t) = H(y)$, then the value of this function remains constant along the solution $y(t)$, that is:

$$H(y(t)) = H(y_0), \qquad \text{for all} \quad t \geq t_0.$$

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In particular, we shall consider the simpler case where

$$H(y) = \frac{1}{2} y^T S y, \qquad S = S^T \in \mathbb{R}^{2m\times 2m}. \tag{2}$$

In this case, problem (1) is linear:

$$y' = J_{2m}^T S y, \quad t \in [t_0, T], \qquad y(t_0) = y_0. \tag{3}$$

In the following, we assume the matrix S to be nonsingular.

Another important feature of problem (3) is that oriented areas are preserved by the flow. This because the exponential $e^{J_{2m}^T S}$ is symplectic, that is:

$$(e^{J_{2m}^T S})^T J_{2m} e^{J_{2m}^T S} = J_{2m}.$$

We now want to look for numerical schemes which satisfy the following two requirements:

1. they define a symplectic map and
2. they preserve the quadratic form (2).

Such methods are usually called *symplectic* or *canonical* integrators.

The known symplectic methods are essentially Runge-Kutta schemes[13,19,20,21], while it seems that they are rare in the class of LMMs. This apparent weakness of LMMs has been recently overcome by using them as Boundary Value Methods (BVMs). We shall recall the main facts about BVMs in Section 2. In Section 3 we shall examine one step methods, while in Section 4 we shall consider multistep methods. In Section 5 we shall analyze three classes of symplectic BVMs and, finally, in Section 6 some numerical examples are reported.

2. Boundary Value Methods

In this section we briefly recall the basic results on BVMs[3,7,8]. Let us then consider the IVP

$$y' = f(t, y), \quad t \in [t_0, T], \qquad y(t_0) = y_0. \tag{4}$$

To approximate its solution, we consider the k-step LMM

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \tag{5}$$

used over the partition

$$t_i = t_0 + ih, \quad i = 0, \cdots, N + k_2 - 1, \qquad h = \frac{T - t_0}{N + k_2 - 1},$$

where $0 \le k_2 < k$. As usual, y_{n+i} and f_{n+i} denote the approximations to $y(t_{n+i})$ and $f(t_{n+i}, y(t_{n+i}))$, respectively. It is known that the discrete problem (5) needs k

independent conditions to be imposed, in order to get the discrete solution. The most commonly used way of imposing such conditions is to fix the values of the discrete solution at the first k grid points, that is one fixes the values $y_0, \cdots, y_{k-1}$. The continuous problem (4) provides only the value y_0, while the remaining ones must be obtained by other means. In other words, the continuous IVP is approximated by means of a discrete IVP. The methods obtained in this way will be called Initial Value Methods (IVMs). This approach is very simple, but suffers of heavy limitations, summarized by the two well-known Dahlquist barriers.

An alternative approach has been considered, where the k conditions needed by the difference equation (5) are imposed by fixing the values

$$y_0, \cdots, y_{k_1-1}, \quad y_N, \cdots, y_{N+k_2-1}, \quad k_1 + k_2 = k. \tag{6}$$

This means that the continuous IVP is now approximated by means of a discrete BVP. The methods obtained in this way have been called BVMs. If the values (6) are fixed, we say that scheme (5) is used with (k_1, k_2)-boundary conditions[7,8,9]. As before, only the value y_0 is provided by the continuous problem, while the remaining values must be obtained in some appropriate way.

For the moment we shall neglect the problem of finding the unknown values in (6). This problem will be considered in Section 2.1.

The definition of 0-stability and Absolute stability for IVMs are now generalized to BVMs by introducing the following two kinds of polynomials.

Definition 1. A polynomial $p(z)$ of degree $k = k_1 + k_2$ is said to be an $S_{k_1k_2}$-*polynomial* if its roots are such that

$$|z_1| \le |z_2| \le \cdots \le |z_{k_1}| < 1 < |z_{k_1+1}| \le \cdots \le |z_k|,$$

while it is called an $N_{k_1k_2}$-*polynomial* if

$$|z_1| \le |z_2| \le \cdots \le |z_{k_1}| \le 1 < |z_{k_1+1}| \le \cdots \le |z_k|,$$

where the roots of unit modulus are simple.

We observe that, for $k_1 = k$ and $k_2 = 0$, $N_{k_1k_2}$-polynomials reduce to Von Neumann polynomials while $S_{k_1k_2}$-polynomials reduce to Schur polynomials. Now we can give the following definitions for BVMs[7−9].

Definition 2. BVM (5) used with (k_1, k_2)-boundary conditions is said to be $0_{k_1k_2}$-*stable* if the polynomial

$$\rho(z) = \sum_{i=0}^{k} \alpha_i z^i$$

is an $N_{k_1k_2}$-polynomial. It is said to be (k_1, k_2)-*Absolutely stable* for a given $q \in \mathbb{C}$ if the polynomial

$$\pi(z, q) = \sum_{i=0}^{k} (\alpha_i - q\beta_i) z^i \tag{7}$$

is an $S_{k_1k_2}$-polynomial. The region

$$\mathcal{D}_{k_1k_2} = \{q \in \mathbb{C} : \pi(z,q) \text{ is an } S_{k_1k_2}\text{-polynomial }\}$$

is called *region of* (k_1,k_2)-*Absolute stability* of the method. Finally, the method is said to be $A_{k_1k_2}$-*stable* if $\mathbb{C}^- \subseteq \mathcal{D}_{k_1k_2}$, where $\mathbb{C}^-$ is the left half of the complex plane.

The given definitions reduce to the well-known ones for IVMs when $k_1 = k$ and $k_2 = 0$. This means that the class of the BVMs contains the IVMs as a proper subclass. Moreover, to fully understand the meaning of the above definitions, especially the definition of (k_1,k_2)-Absolute stability, we report without proof the following result[8]. It will be re-derived in a more general form in Section 4.

We need the following notations: let

$$|z_1| \leq \cdots \leq |z_k|$$

be the roots of polynomial (7), relative to the use of method (5) on the usual test equation:

$$y' = \lambda y, \quad y(t_0) = y_0, \quad q = h\lambda. \tag{8}$$

Then, the following result holds true.

Theorem 1. *Let*

$$|z_{k_1-1}| < |z_{k_1}| < |z_{k_1+1}|, \quad |z_{k_1-1}| < 1 < |z_{k_1+1}|.$$

Then, the discrete solution of method (5), *used with* (k_1,k_2)-*boundary conditions, is given by:*

$$\begin{aligned} y_n =& z_{k_1}^n(\gamma + O(|z_{k_1}/z_{k_1+1}|^{N-n}) + O(|z_{k_1+1}|^{-N})) \\ &+ O(|z_{k_1-1}|^n) + O(|z_{k_1+1}|^{-(N-n)}), \end{aligned} \tag{9}$$

where γ *depends only on the initial conditions.*

The above result states that the numerical solution is essentially generated by the root z_{k_1}, which therefore will be called *generating root*[8]. Moreover, we observe that $|z_{k_1}| < 1$, if $q \in \mathcal{D}_{k_1k_2}$.

From (8) and (9), it follows that the discrete solution will be an effective approximation of the continuous one when z_{k_1} is the principal root of the method. In this case, if the method has order p, one has:

$$z_{k_1} \equiv z_{k_1}(q) = e^q + O(h^{p+1}).$$

For this purpose, the next result holds true.

Theorem 2. *If a k-step LMM, used with* (k_1,k_2)-*boundary conditions on problem* (8), *is:*

1. *consistent,*

2. $0_{k_1k_2}$-*stable, and*

3. *the associated polynomial* $\rho(z)$ *has only one root of unit modulus* (*i.e.* $z = 1$),

then there is a neighborhood D *of* $q = 0$ *where the generating root of the method coincides with its principal root. In this case, the constant* γ *in* (9) *is given by* $\gamma = y_0 + O(h^p)$, *provided that the additional initial conditions are at least* $O(h^p)$ *accurate.*

Proof. See [8].

The advantage of BVMs over IVMs is that now there are no more barriers concerning the order of $0_{k_1k_2}$-stable and $A_{k_1k_2}$-stable methods. In fact, in Section 5 we shall consider $0_{k_1k_2}$-stable, $A_{k_1k_2}$-stable methods of order up to $2k$, for every odd k.

2.1. The additional conditions

Let us rewrite scheme (5), used with (k_1, k_2)-boundary conditions by fixing the values (6), as follows:

$$\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i}, \quad n = k_1, \cdots, N-1. \tag{10}$$

Thus, we have a set of $N - k_1$ equations in the $N - k_1$ unknowns $y_{k_1}, \cdots, y_{N-1}$. It follows that if the values (6) are really known, then we can obtain the discrete solution.

However, the only value provided by the continuous problem is the initial condition y_0. It follows that we must regard the remaining $k-1$ values $y_1, \cdots, y_{k_1-1}$, $y_N, \cdots, y_{N+k_2-1}$ as unknowns. This implies that we must add an additional set of $k-1$ equations independent of those in (10). These equations can be derived by suitable methods of order (at least) $p-1$, in order to preserve the global error of the method[8].

Each of the methods presented in the next sections, will be associated with an appropriate set of additional equations.

3. One-step Methods

We start considering the case of one-step methods. We shall assume the method to be consistent, so that its form will be:

$$y_{n+1} - y_n = h(\beta_1 f_{n+1} + \beta_0 f_n). \tag{11}$$

Since this method requires only one condition to be imposed, it will be an IVM. When we apply this scheme to problem (3), then the discrete solution is given by:

$$(I - h\beta_1 J_{2m}^T S) y_{n+1} = (I + h\beta_0 J_{2m}^T S) y_n,$$

that is, if we assume the matrix $(I - h\beta_1 J_{2m}^T S)$ to be nonsingular,

$$\begin{aligned} y_{n+1} &= (I - h\beta_1 J_{2m}^T S)^{-1} (I + h\beta_0 J_{2m}^T S) y_n \\ &=: \varphi(hJ_{2m}^T S) y_n \equiv \varphi(hJ_{2m}^T S)^{n+1} y_0. \end{aligned} \tag{12}$$

Then, the method will be symplectic if

$$\varphi(hJ_{2m}^T S)^T J_{2m} \varphi(hJ_{2m}^T S) = J_{2m},$$

and

$$y_{n+1}^T S y_{n+1} = y_n^T S y_n.$$

In this case, the following theorem due to Feng[11,13,14] can be used.

Theorem 3. *Let $\varphi(z)$ be a complex valued function such that:*

1. *$\varphi(z)$ is analytical and with real coefficients in a neighborhood D of $z = 0$;*

2. *$\varphi(z)\varphi(-z) \equiv 1$ in D;*

3. *$\varphi'(0) \neq 0$.*

Then, for all square matrices C and L, one has $\varphi(hL)^T C \varphi(hL) = C$ iff $C\,L + L^T C = O$.

When $C = J_{2m}$, then $\varphi(hL)$ is symplectic iff L is Hamiltonian. Moreover, if in this case $L = J_{2m}^T S$, $S = S^T$, then one also has:

$$SL + L^T S = SJ_{2m}^T S + SJ_{2m} S = O,$$

so that

$$\varphi(hL)^T S \varphi(hL) = S$$

follows. The above relation implies the conservation of the quadratic form (2) for the discrete sequence defined by:

$$y_{n+1} = \varphi(hL) y_n.$$

Coming back to method (11), we observe that the iteration function $\varphi(z)$ defined in (12) is given by:

$$\varphi(z) = \frac{1 + \beta_0 z}{1 - \beta_1 z}.$$

This function is evidently analytical and with real coefficients in a neighborhood D of $z = 0$. Moreover, it is:

$$\varphi'(0) = \beta_0 + \beta_1 = \sigma(1) = \rho'(1) \neq 0,$$

so that the hypotheses 1) and 3) of Feng's Theorem are fulfilled. It remains to satisfy condition 2), which reads as follows:

$$\frac{1 + \beta_0 z}{1 - \beta_1 z} = \frac{1 + \beta_1 z}{1 - \beta_0 z},$$

thus giving $\beta_0 = \beta_1$. From the consistency conditions, it follows that $\beta_0 = \beta_1 = \dfrac{1}{2}$, so that the well-known trapezoidal rule is obtained:

$$y_{n+1} - y_n = \frac{h}{2}(f_{n+1} + f_n).$$

This is, therefore, a symplectic method. This is a known result[11]. We shall extend this result to general multistep methods with higher number of steps in the next section.

4. Multistep Methods

Let us consider the k-step method (5), to be used with (k_1, k_2)-boundary conditions. In the following, we shall assume that the method is irreducible, of order $p \geq 1$, and satisfying the hypotheses of Theorem 2. Then, there exists a neighborhood D of $q = 0$ where the generating root of the method, z_{k_1}, coincides with the principal one.

Moreover, let

$$\pi(z, q) = \rho(z) - q\sigma(z), \quad q = h\lambda, \tag{13}$$

be its characteristic polynomial, whose roots are ordered by increasing moduli:

$$|z_1| \leq \cdots \leq |z_k|.$$

To examine the properties of this method when used on problem (3), we need to generalize the result of Theorem 1. To do this, we start analyzing the application of the method to the following problem:

$$y' = J_\lambda y, \quad t \in [t_0, T], \quad y(t_0) = y_0,$$

where the vector $y \in \mathbb{C}^m$, and

$$J_\lambda = \begin{pmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix}_{m\times m}. \tag{14}$$

Let $h = (T - t_0)/(N + k_2 - 1)$ be the used stepsize. Then, for each root $z_j = z_j(h\lambda)$, $j = 1, \cdots, k$, of polynomial (13), we define the matrix:

$$S_j := z_j(hJ_\lambda) = \begin{pmatrix} z_j(q) & hz_j(q)' & \cdots & \dfrac{h^{m-1}z_j(q)^{(m-1)}}{(m-1)!} \\ & \ddots & \ddots & \vdots \\ & & \ddots & hz_j(q)' \\ & & & z_j(q) \end{pmatrix}_{m\times m}. \tag{15}$$

Then, the following result holds true.

Lemma 1. *Let the method* (5) *satisfy the hypotheses of Theorem* 1. *Moreover, suppose the roots of $\pi(z, h\lambda)$ to be simple. Then the discrete solution provided by the method behaves, for n and $N - n$ large, as:*

$$y_n = S_{k_1}^n(y_0 + d(n, N, h))) + g(n, N, h). \tag{16}$$

The quantities $d(n, N, h)$ and $g(n, N, h)$ are defined as follows:

1. $d(n, N, h) = O(h^p)$, $g(n, N, h) = O(h^p)(O(|z_{k_1-1}|^n) + O(|z_{k_1+1}|^{n-N}))$, *in the case where z_{k_1} is the principal root of the method and the additional conditions have at least $O(h^p)$ accuracy;*

2. $d(n,N,h) = v + O(|z_{k_1}/z_{k_1+1}|^{N-n}) + O(|z_{k_1+1}|^{-N})$, $g(n,N,h) = O(|z_{k_1-1}|^n) + O(|z_{k_1+1}|^{n-N})$, *with the vector* v *depending only on the initial conditions, otherwise.*

Proof. In the following, we shall denote as case 1) the case where z_{k_1} is the principal root of the method and the additional conditions have at least $O(h^p)$ accuracy.

Since we have assumed the roots $\{z_i\}$ to be simple, it follows that the matrices $\{S_1, \cdots, S_k\}$ constitute a complete set of solvents[15] for the matrix polynomial

$$\rho(z)I_m - hJ_\lambda \sigma(z).$$

Then, the discrete solution provided by the method (5) can be written as:

$$y_n = \sum_{j=1}^{k} S_j^n c_j,$$

where the vectors $\{c_j\}$ are determined by fixing the values

$$y_0, y_1, \cdots, y_{k_1-1}, y_N, \cdots, y_{N+k_2-1}$$

of the discrete solution. This can be recast in matrix form as follows:

$$M \begin{pmatrix} c_{k_1} \\ \mathbf{c}_i \\ \mathbf{c}_f \end{pmatrix} = \begin{pmatrix} y_0 \\ \mathbf{y}_i \\ \mathbf{y}_f \end{pmatrix},$$

where:

$$\mathbf{c}_i = \begin{pmatrix} c_1 \\ \vdots \\ c_{k_1-1} \end{pmatrix}, \quad \mathbf{c}_f = \begin{pmatrix} c_{k_1+1} \\ \vdots \\ c_k \end{pmatrix}, \quad \mathbf{y}_i = \begin{pmatrix} y_1 \\ \vdots \\ y_{k_1-1} \end{pmatrix}, \quad \mathbf{y}_f = \begin{pmatrix} y_N \\ \vdots \\ y_{N+k_2-1} \end{pmatrix},$$

and

$$M = \begin{pmatrix} I_m & E_{k_1-1}^T & E_{k_2}^T \\ W_{k_1-1}S_{k_1} & U_{k_1-1}D_i & V_{k_1-1}D_f \\ W_{k_2}S_{k_1}^N & U_{k_2}D_i^N & V_{k_2}D_f^N \end{pmatrix},$$

$$W_j = \begin{pmatrix} I_m \\ S_{k_1} \\ \vdots \\ S_{k_1}^{j-1} \end{pmatrix}, \qquad E_j = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}_{j\times 1} \otimes I_m,$$

$$U_j = \begin{pmatrix} I_m & \cdots & I_m \\ S_1 & \cdots & S_{k_1-1} \\ \vdots & & \vdots \\ S_1^{j-1} & \cdots & S_{k_1-1}^{j-1} \end{pmatrix}, \qquad D_i = \begin{pmatrix} S_1 & & \\ & \ddots & \\ & & S_{k_1-1} \end{pmatrix},$$

$$V_j = \begin{pmatrix} I_m & \cdots & I_m \\ S_{k_1+1} & \cdots & S_k \\ \vdots & & \vdots \\ S_{k_1+1}^{j-1} & \cdots & S_k^{j-1} \end{pmatrix}, \quad D_f = \begin{pmatrix} S_{k_1+1} & & \\ & \ddots & \\ & & S_k \end{pmatrix}.$$

After some calculations, one finds that

$$M^{-1} = \begin{pmatrix} (I_m + E_{k_1-1}^T B_1^{-1} W_{k_1-1} S_{k_1} + F\,H) & (F\,B_2 - E_{k_1-1}^T) B_1^{-1} & -F \\ B_1^{-1}(C\,G^{-1}H - W_{k_1-1}S_{k_1}) & B_1^{-1}(\hat{I}_i + C\,G^{-1}B_2 B_1^{-1}) & -B_1^{-1}C\,G^{-1} \\ -G^{-1}H & -G^{-1}B_2 B_1^{-1} & G^{-1} \end{pmatrix},$$

where:

$$\begin{aligned} \hat{I}_i &= I_{k_1-1} \otimes I_m, \\ B_1 &= U_{k_1-1} D_i - W_{k_1-1} S_{k_1} E_{k_1-1}^T, \\ B_2 &= U_{k_2} D_i^N - W_{k_2} S_{k_1}^N E_{k_1-1}^T, \\ C &= V_{k_1-1} D_f - W_{k_1-1} S_{k_1} E_{k_2}^T, \\ G &= V_{k_2} D_f^N - W_{k_2} S_{k_1} E_{k_2}^T - B_2 B_1^{-1} C \\ &= (V_{k_2} + O(|z_{k_1+1}|^{-N})) D_f^N, \\ F &= (E_{k_2}^T - E_{k_1-1}^T B_1^{-1} C) G^{-1} \\ &= (E_{k_2}^T - E_{k_1-1}^T B_1^{-1} C) D_f^{-N} (V_{k_2} + O(|z_{k_1+1}|^{-N}))^{-1}, \\ H &= W_{k_2} S_{k_1}^N - B_2 B_1^{-1} W_{k_1-1} S_{k_1}. \end{aligned}$$

Moreover, by denoting with

$$\boldsymbol{\xi}_i(h) = \mathbf{y}_i - W_{k_1-1} S_{k_1} y_0, \quad \boldsymbol{\xi}_f(h) = \mathbf{y}_f - W_{k_1-1} S_{k_1}^N y_0,$$

one has that

$$\boldsymbol{\xi}_i(h) = \begin{cases} O(h^p), & \text{in case 1)}, \\ O(1), & \text{otherwise}, \end{cases} \quad \boldsymbol{\xi}_f(h) = \begin{cases} O(h^p), & \text{in case 1)}, \\ O(|z_{k_1}|^N), & \text{otherwise}. \end{cases}$$

This allows us to derive the unknown vectors $\{c_j\}$ as follows:

$$\begin{aligned} c_{k_1} &= y_0 + E_{k_1-1}^T B_1^{-1} \boldsymbol{\xi}_i(h) + F(B_2 B_1^{-1} \boldsymbol{\xi}_i(h) - \boldsymbol{\xi}_f(h)) \\ &= \begin{cases} y_0 + O(h^p), & \text{in case 1)}, \\ y_0 + v + O(|z_{k_1}/z_{k_1+1}|^N) + O(|z_{k_1+1}|^{-N}), & \text{otherwise}, \end{cases} \end{aligned}$$

where the vector $v = E_{k_1-1}^T B_1^{-1} \boldsymbol{\xi}_i(h)$ depends, obviously, only on the initial conditions. Similarly, we obtain:

$$\begin{aligned} \mathbf{c}_i &= B_1^{-1}((\hat{I}_i + CG^{-1}B_2 B_1^{-1})\boldsymbol{\xi}_i(h) - CG^{-1}\boldsymbol{\xi}_f(h)) \\ &= \begin{cases} O(h^p), & \text{in case 1)}, \\ O(1), & \text{otherwise}, \end{cases} \end{aligned}$$

and, finally,

$$\mathbf{c}_f = G^{-1}(\boldsymbol{\xi}_f(h) - B_2 B_1^{-1}\boldsymbol{\xi}_i(h)) = \begin{cases} D_f^{-N} O(h^p), & \text{in case 1),} \\ D_f^{-N}(O(1) + O(|z_{k_1}|^N)), & \text{otherwise.} \end{cases}$$

From the above relations, one finally obtains:

$$\begin{aligned} y_n &= S_{k_1}^n c_{k_1} + D_i^n \mathbf{c}_i + D_f^n \mathbf{c}_f^n \\ &= \begin{cases} S_{k_1}^n (y_0 + O(h^p)) + O(h^p) O(|z_{k_1-1}|^n) + \\ \qquad O(h^p) O(|z_{k_1+1}|^{n-N}), & \text{in case 1),} \\ S_{k_1}^n (y_0 + v + O(|z_{k_1}/z_{k_1+1}|^{N-n}) + O(|z_{k_1+1}|^{-N})) + \\ \quad O(|z_{k_1-1}|^n) + O(|z_{k_1+1}|^{n-N}), & \text{otherwise.} \end{cases} \end{aligned}$$

Observe that when $m = 1$, we obtain the result of Theorem 1. Moreover, we observe that from (16) one has that the discrete solution is now essentially generated by the matrix S_{k_1}. This matrix will be called *generating matrix*, in analogy with the scalar case.

We now apply the result of the previous lemma to the adjoint equation:

$$y' = -J_\lambda^T y, \quad t \in [t_0, T], \qquad y(t_0) = y_0,$$

where J_λ is given by (14). The following result holds true.

Lemma 2. *Let method* (5) *satisfy the hypotheses of Theorem* 1, *with* $k_1 = \nu$ *and* $k_2 = \nu - 1$. *Moreover, let the roots of the polynomial* $\pi(z, h\lambda)$ *be simple, and the polynomials* $\rho(z)$ *and* $\sigma(z)$ *satisfy the following requirements:*

$$\rho(z) = -z^k \rho(z^{-1}), \quad \sigma(z) = z^k \sigma(z^{-1}). \tag{17}$$

Then, the generating matrix of the method is given by S_ν^{-T}, *where* S_ν *is given by* (15), *with* $j = \nu$.

Proof. First of all, we observe that if the polynomials $\rho(z)$ and $\sigma(z)$ of the method satisfy relation (17), then

$$\pi(\xi, q) := \rho(\xi) - q\sigma(\xi) = 0 \quad \text{iff} \quad \pi(\xi^{-1}, -q) := \rho(\xi^{-1}) + q\sigma(\xi^{-1}) = 0.$$

It follows that if $\xi(q)$ is one of the roots, then one has:

$$\xi(-q) = \xi(q)^{-1}. \tag{18}$$

Moreover, method (5) satisfies the hypotheses of Lemma 1. Then, by using arguments similar to those used in the proof of that Lemma, we have that the generating matrix needs to be $z_\nu(-hJ_\lambda)^T$. The thesis then completes by observing that from (18) one has

$$z_\nu(-hJ_\lambda)^T = z_\nu(hJ_\lambda)^{-T} \equiv S_\nu^{-T}.$$

Let us now consider the application of method (5), used with (k_1, k_2)-boundary conditions, to problem (3). If the symmetric matrix S is real and nonsingular, then, by using arguments similar to those used in [16], it is possible to find a (generally complex) matrix V such that

$$V^T J_{2m} V = J_{2m}, \quad V^{-1} J_{2m}^T S V = \begin{pmatrix} J_{\lambda_1} & & & & & \\ & \ddots & & & & \\ & & J_{\lambda_r} & & & \\ & & & -J_{\lambda_1}^T & & \\ & & & & \ddots & \\ & & & & & -J_{\lambda_r}^T \end{pmatrix} =: \Lambda, \quad (19)$$

where $\pm\lambda_1, \cdots, \pm\lambda_r$ are the eigenvalues (not necessarily distinct) of $J_{2m}^T S$, and

$$J_{\lambda_i} = \begin{pmatrix} \lambda_i & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{pmatrix}_{m_i \times m_i}, \quad i = 1, \cdots, r.$$

Moreover, for $i = 1, \cdots, r$, let

$$|z_1^{(i)}| \leq \cdots \leq |z_k^{(i)}| \quad (20)$$

be the roots of the polynomial

$$\pi(z, q_i) = \rho(z) - q_i \sigma(z), \qquad q_i = h\lambda_i,$$

and

$$|\hat{z}_1^{(i)}| \leq \cdots \leq |\hat{z}_k^{(i)}| \quad (21)$$

those of

$$\pi(z, -q_i) = \rho(z) + q_i \sigma(z).$$

If method (5) satisfies the hypotheses of Theorem 2 and moreover for all $i = 1, \cdots, r$:

a) the roots $\{z_j^{(i)}\}$ and $\{\hat{z}_j^{(i)}\}$ are all simple, and

b) $\begin{cases} |z_{k_1-1}^{(i)}| < |z_{k_1}^{(i)}| < |z_{k_1+1}^{(i)}|, & |z_{k_1-1}^{(i)}| < 1 < |z_{k_1+1}^{(i)}|, \\ |\hat{z}_{k_1-1}^{(i)}| < |\hat{z}_{k_1}^{(i)}| < |\hat{z}_{k_1+1}^{(i)}|, & |\hat{z}_{k_1-1}^{(i)}| < 1 < |\hat{z}_{k_1+1}^{(i)}|, \end{cases}$

then the discrete solution is given by

$$y_n = Z^n(y_0 + d(n, N, h)) + g(n, N, h).$$

In the above expression,

$$Z = V \begin{pmatrix} z_{k_1}^{(1)}(hJ_{\lambda_1}) & & & & & \\ & \ddots & & & & \\ & & z_{k_1}^{(r)}(hJ_{\lambda_r}) & & & \\ & & & \hat{z}_{k_1}^{(1)}(-hJ_{\lambda_1})^T & & \\ & & & & \ddots & \\ & & & & & \hat{z}_{k_1}^{(r)}(-hJ_{\lambda_r})^T \end{pmatrix} V^{-1}, =: V\hat{Z}V^{-1}, \quad (22)$$

and, by denoting with

$$\eta = \min_i\{|z^{(i)}_{k_1+1}|, |\hat z^{(i)}_{k_1+1}|\},\ \zeta = \max_i\{|z^{(i)}_{k_1-1}|, |\hat z^{(i)}_{k_1-1}|\},\ \mu = \max_i\{|z^{(i)}_{k_1}/z^{(i)}_{k_1+1}|, |\hat z^{(i)}_{k_1}/\hat z^{(i)}_{k_1+1}|\},$$

1. $d(n,N,h) = O(h^p), \quad g(n,N,h) = O(h^p)(O(\zeta^n) + O(\eta^{n-N}))$,

   if all the roots $\{z^{(i)}_{k_1}\}$ and $\{\hat z^{(i)}_{k_1}\}$ are principal roots (i.e. $z^{(i)}_{k_1} = e^{h\lambda_i} + O(h^{p+1})$ and $\hat z^{(i)}_{k_1} = e^{-h\lambda_i} + O(h^{p+1})$, for all $i = 1,\cdots,r$) and, moreover, the additional conditions are at least $O(h^p)$ accurate;

2. $d(n,N,h) = v + O(\mu^{N-n}) + O(\eta^{-N}), \quad g(n,N,h) = O(\zeta^n) + O(\eta^{n-N})$,

   where the vector v depends only on the initial conditions, otherwise.

This can be proved by using the result of Lemma 1 on each subproblem of the transformed equation

$$\hat y' = \Lambda \hat y, \qquad \hat y = V^{-1} y.$$

Concerning the previous requirements a) and b), we can say that they are fulfilled almost everywhere. In fact, concerning requirement a), if ξ is a multiple root of the polynomial $\rho(z) - q\sigma(z)$, then we have:

$$\rho(\xi) - q\sigma(\xi) = \rho'(z) - q\sigma'(q) = 0,$$

that is,

$$\frac{\rho(\xi)}{\sigma(\xi)} = \frac{\rho'(\xi)}{\sigma'(\xi)}.$$

It follows that multiple roots may occur only in correspondence of the (at most) $2k-1$ roots of the polynomial:

$$\rho(z)\sigma'(z) - \rho'(z)\sigma(z).$$

On the other hand, concerning requirement b), it is possible to show that roots of equal modulus may occur at most over a set of zero measure, in the q-plane. Moreover, this set does not contain the origin, if the hypotheses of Theorem 2 are satisfied, as we have assumed.

Then, we may say that the numerical solution originated by method (5) is essentially generated by the matrix Z defined in (22). This justifies the following definition.

Definition 3. The method (5) is "essentially" symplectic if Z is a symplectic matrix and, moreover,

$$Z^T S Z = S, \tag{23}$$

thus giving that the quadratic form (2) is "essentially" preserved by the discrete solution.

Moreover, in this case also the quantity

$$e(h) = \max_n |H(y(t_n)) - H(y_n)| \tag{24}$$

essentially depends only on the stepsize h, and not on the number of the mesh points, that is, on the length of the interval of integration $T - t_0$. In particular, it follows that, for essentially symplectic methods, $e(h)$ is always $O(h^p)$, if all the zeros $\{z_{k_1}^{(i)}\}$ and $\{\hat{z}_{k_1}^{(i)}\}$ are principal roots and the values (6) have at least $O(h^p)$ accuracy.

Let us then concentrate ourselves on the conditions which allow to obtain a matrix Z which is symplectic and satisfies equation (23). The following result holds true.

Theorem 4. *Let the method* (5) *satisfy the hypotheses of Lemma* 2. *Then the method is essentially symplectic.*

Proof. Obviously, the matrix Z needs to be real, if the original problem is real. We start showing that

$$Z^T J_{2m} Z = J_{2m}.$$

Since in equation (22) we already have that $V^T J_{2m} V = V^{-T} J_{2m} V^{-1} = J_{2m}$, it suffices to show that $\hat{Z}^T J_{2m} \hat{Z} = J_{2m}$.

Since $k_1 = \nu = k_2 + 1$, from Lemma 2 it follows that for all $i = 1, \cdots, r$, one has:

$$\hat{z}_\nu^{(i)} \equiv z_\nu^{(i)}(-h\lambda_i) = z_\nu^{(i)}(h\lambda_i)^{-1} \equiv (z_\nu^{(i)})^{-1},$$

so that

$$\hat{z}_\nu^{(i)}(-hJ_{\lambda_i}) = \left(z_\nu^{(i)}(hJ_{\lambda_i})\right)^{-1}.$$

Then, from (22) one has:

$$\hat{Z} = \begin{pmatrix} z_\nu^{(1)}(hJ_{\lambda_1}) & & & & & \\ & \ddots & & & & \\ & & z_\nu^{(r)}(hJ_{\lambda_r}) & & & \\ & & & (z_\nu^{(1)}(hJ_{\lambda_1}))^{-T} & & \\ & & & & \ddots & \\ & & & & & (z_\nu^{(r)}(hJ_{\lambda_r}))^{-T} \end{pmatrix}.$$

It is an easy matter to verify that:

$$\hat{Z}^T J_{2m} \hat{Z} = J_{2m}.$$

It remains to show that

$$Z^T S Z = S.$$

From (19) and (22) one has:

$$V(\rho(\hat{Z}) - h\Lambda\sigma(\hat{Z}))V^{-1} = \rho(Z) - hJ_{2m}^T S\sigma(Z) = O.$$

Moreover, since we have assumed the method to be irreducible, $\rho(z)$ and $\sigma(z)$ do not have common factors. It follows that the matrix $\sigma(Z)$ must be nonsingular, thus giving:

$$S = \frac{J_{2m}}{h}\rho(Z)\sigma(Z)^{-1}.$$

By using this relation, and the fact that Z is symplectic, one finally obtains:

$$\begin{aligned} Z^T S Z &= Z^T \frac{J_{2m}}{h}\rho(Z)\sigma(Z)^{-1} Z = Z^T J_{2m} Z \frac{1}{h}\rho(Z)\sigma(Z)^{-1} \\ &= \frac{J_{2m}}{h}\rho(Z)\sigma(Z)^{-1} = S. \end{aligned}$$

5. Essentially Symplectic BVMs

In this section, we introduce three families of essentially symplectic BVMs. Common features to all these methods are the following[8]:

1. they are consistent and irreducible;
2. the corresponding characteristic polynomials $\rho(z)$ and $\sigma(z)$ satisfy (17);
3. they have an odd number of steps: $k = 2\nu - 1$;
4. they must be used with $(\nu, \nu-1)$-boundary conditions, and satisfy the hypotheses of Theorem 2;
5. for all of them, the region of $(\nu, \nu-1)$-Absolute stability coincides with the left half of the complex plane, $\mathbb{C}^-$, so that they are $A_{\nu,\nu-1}$-stable;
6. they can be used for approximating both initial and boundary value problems [9].

Let us briefly examine these three families of methods.

5.1. Extended Trapezoidal Rules

The Extended Trapezoidal Rules (ETRs)[3] have the following form:

$$y_n - y_{n-1} = h \sum_{i=-\nu}^{\nu-1} \beta_{i+\nu} f_{n+i}, \quad \nu = 1, 2, \cdots. \tag{25}$$

The coefficients $\{\beta_i\}$ are uniquely determined by imposing that the method has the highest possible order, that is $p = k + 1 = 2\nu$. It is possible to prove that these coefficients are symmetric[3,8]:

$$\beta_i = \beta_{2\nu-1-i}, \quad i = 0, \cdots, 2\nu - 1,$$

so that the symmetry requirements (17) are satisfied. Scheme (25) is used with $(\nu, \nu-1)$-boundary conditions. It follows that if it is used for $n = \nu, \cdots, N-1$, then the following additional equations can be considered for the additional conditions:

$$y_r - y_{r-1} = h \sum_{i=0}^{2\nu-2} \beta_{i,r} f_i, \quad r = 1, \cdots, \nu - 1, \tag{26}$$

and

$$y_r - y_{r-1} = h \sum_{i=0}^{2\nu-2} \beta_{i,r} f_{N-\nu+i}, \quad r = N, \cdots, N + \nu - 2. \tag{27}$$

In each case, the coefficients $\{\beta_{i,r}\}$ are uniquely determined by imposing the corresponding formula to have order $k = 2\nu - 1$ [9].

Example 1.

When $\nu = 1$, formula (25) reduces to the usual trapezoidal rule, which is the simplest ETR and does not need additional equations.

For $\nu = 2$, we get the ETR of order four:

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

It can be used with the following two additional equations:

$$y_1 - y_0 = \frac{h}{12}(-f_2 + 8f_1 + 5f_0),$$

and

$$y_N - y_{N-1} = \frac{h}{12}(5f_N + 8f_{N-1} - f_{N-2}).$$

For $\nu = 2$, we obtain the ETR of order six:

$$y_n - y_{n-1} = \frac{h}{1440}(11f_{n+2} - 93f_{n+1} + 802f_n + 802f_{n-1} - 93f_{n-2} + 11f_{n-3}), \quad n = 3, \cdots, N-1.$$

It can be used with the following four additional equations:

$$\begin{aligned}
y_1 - y_0 &= \frac{h}{720}(-19f_4 + 106f_3 - 264f_2 + 646f_1 + 251f_0), \\
y_2 - y_1 &= \frac{h}{720}(11f_4 - 74f_3 + 456f_2 + 346f_1 - 19f_0), \\
y_N - y_{N-1} &= \frac{h}{720}(-19f_{N+1} + 346f_N + 456f_{N-1} - 74f_{N-2} + 11f_{N-3}), \\
y_{N+1} - y_N &= \frac{h}{720}(251f_{N+1} + 646f_N - 264f_{N-1} + 106f_{N-2} - 19f_{N-3}).
\end{aligned}$$

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 a new class of methods which preserve the structure of the second characteristic polynomial, $\sigma(z)$, of the trapezoidal rule. The following methods, which we call Extended Trapezoidal Rules of second kind (ETR$_2$s), are then obtained:

$$\sum_{i=-\nu}^{\nu-1} \alpha_{i+\nu} y_{n+i} = \frac{h}{2}(f_n + f_{n-1}). \tag{28}$$

As in the case of ETRs, the coefficients $\{\alpha_i\}$ are uniquely determined by imposing that the method has the highest possible order, that is $p = k + 1 = 2\nu$. It is possible to prove that these coefficients are skew-symmetric[8]:

$$\alpha_i = -\alpha_{2\nu-1-i}, \quad i = 0, \cdots, 2\nu - 1,$$

so that the symmetry requirements (17) are satisfied for these methods. Formula (28) is used with $(\nu, \nu-1)$-boundary conditions. It follows that if we use it for $n = \nu, \cdots, N-1$, then the following additional equations can be considered for the additional conditions:

$$\sum_{i=0}^{2\nu-1} \alpha_{i,r} y_i = \frac{h}{2}(f_r + f_{r-1}), \quad r = 1, \cdots, \nu - 1.$$

and

$$\sum_{i=0}^{2\nu-1} \alpha_{i,r} y_{N-\nu-1+i} = \frac{h}{2}(f_r + f_{r-1}), \quad r = N, \cdots, N + \nu - 2.$$

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

Example 2.

When $\nu = 1$, from formula (28) we find again the trapezoidal rule, which also is the simplest ETR_2.

For $\nu = 2$ we obtain the following fourth order ETR_2:

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

In this case, the two required additional equations can be chosen as follows:

$$\begin{aligned} &\frac{1}{12}(y_3 - 3y_2 + 15y_1 - 13y_0) = \frac{h}{2}(f_1 + f_0,), \\ &\frac{1}{12}(13y_N - 15y_{N-1} + 3y_{N-2} - y_{N-3}) = \frac{h}{2}(f_N + f_{N-1},). \end{aligned}$$

For $\nu = 3$ we obtain the sixth order ETR_2:

$$\frac{1}{120}(- y_{n+2} + 15y_{n+1} + 80y_n - 80y_{n-1} - 15y_{n-2} + y_{n-3}) = \frac{h}{2}(f_n + f_{n-1},).$$

It can be used with the following set of additional equations:

$$\begin{aligned} &\frac{1}{120}(9y_5 - 55y_4 + 140y_3 - 180y_2 + 235y_1 - 149y_0) = \frac{h}{2}(f_1 + f_0), \\ &\frac{1}{120}(- y_5 + 5y_4 + 100y_2 - 95y_1 - 9y_0) = \frac{h}{2}(f_2 + f_1), \\ &\frac{1}{120}(9y_{N+1} + 95y_N - 100y_{N-1} - 5y_{N-3} + y_{N-4}) = \frac{h}{2}(f_N + f_{N-1}), \\ &\frac{1}{120}(149y_{N+1} - 235y_N + 180y_{N-1} - 140y_{N-2} + 55y_{N-3} - 9y_{N-4}) = \frac{h}{2}(f_{N+1} + f_N). \end{aligned}$$

5.3. Top Order Methods

The last family of methods we consider is that of Top Order Methods (TOMs). The name of these methods[1,8] derives from the fact that the coefficients of the generic k-step $(k = 2\nu - 1)$ method in this class

$$\sum_{i=-\nu}^{\nu-1} \alpha_{i+\nu} y_{n+i} = h \sum_{i=-\nu}^{\nu-1} \beta_{i+\nu} f_{n+i}, \tag{29}$$

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

Formula (29) is used with $(\nu, \nu-1)$-boundary conditions. It follows that if we use it for $n = \nu, \cdots, N-1$, then suitable methods of order $2k-1$ must be used to obtain the required $2\nu - 2$ additional equations (for more details[8,9]).

Example 3.

When $\nu = 1$, from formula (29) we reobtain the trapezoidal rule, which is the simplest TOM.

For $\nu = 2$, 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, if used for $n = 2, \cdots, N-1$, requires two additional equations. These can be chosen as follows:

$$\frac{1}{210}(52y_3 + 81y_2 - 108y_1 - 25y_0) = \frac{h}{70}(2f_3 + 27f_2 + 36f_1 + 5f_0),$$

and

$$\frac{1}{210}(25y_N + 108y_{N-1} - 81y_{N-2} - 52y_{N-3}) = \frac{h}{70}(5f_N + 36f_{N-1} + 27f_{N-2} + 2f_{N-3}).$$

These equations are obtained by two methods of order five.

5.4. Nonlinear Problems

We have seen that essentially symplectic LMMs exist for linear Hamiltonian systems. However, in general we can not state that they also have the same properties when used on nonlinear problems. Nevertheless, even in this case something can be said. In fact, suppose that

$$y' = f(y)$$

is a given nonlinear autonomous Hamiltonian system, and to use a k-step essentially symplectic integrator to approximate its solution. We obtain:

$$\rho(E)y_n - h\sigma(E)f(y_n) = 0, \tag{30}$$

where the polynomials $\rho(z)$ and $\sigma(z)$ satisfy the hypotheses of Theorem 4. In this case, it is known [10] that the one-leg twin:

$$\rho(E)y_n - hf(\sigma(E)y_n) = 0, \tag{31}$$

defines a symplectic map with respect to the matrix

$$M \otimes J_{2m},$$

where M is a $k \times k$ matrix which depends only on the coefficients of the method. Moreover, from equation (31), the following set of equations are readily obtained:

$$\beta_i(\rho(E)y_{n+i} - hf(\sigma(E)y_{n+i})) = 0, \quad i = 0, \cdots, k,$$

where the $\{\beta_i\}$ are, as usual, the coefficients of the polynomial $\sigma(z)$. Suppose to use the scaling $\sigma(1) = 1$. Then, by calling

$$\hat{y}_n = \sigma(E) y_n,$$

it follows that

$$\rho(E)\hat{y}_n - h\sigma(E) f(\hat{y}_n) = 0,$$

that is the new "averaged" variable $\hat{y}_n$ satisfies equation (30). It follows that we can expect method (30) to share many of the properties of its one-leg twin (31). Moreover, its order is in general higher.

6. Numerical Examples

Let us consider the following linear Hamiltonian problem:

$$y' = \begin{pmatrix} 0 & 10 \\ -1 & 0 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 2 \end{pmatrix}. \tag{32}$$

The Hamiltonian function is:

$$H(y) = \frac{1}{2} y^T \begin{pmatrix} 1 & 0 \\ 0 & 10 \end{pmatrix} y.$$

In the following Table 1, we report the computed values of $e(h)$ (see [24]). We want to stress that this maximum value essentially depends only on the stepsize h used to obtain the mesh, rather than on the number of mesh points, as we said in Section 4. The labels ETR4 and $\text{ETR}_2 4$ denote the fourth order ETR and the corresponding formula of second kind, respectively. Finally, TOM6 denotes the sixth order TOM.

Table 1 Numerical results relative to problem (32)

	ETR4		$\text{ETR}_2 4$		TOM6	
h	$e(h)$	rate	$e(h)$	rate	$e(h)$	rate
0.1	3.360e-2	–	2.970e-2	–	6.705e-04	–
0.05	2.127e-3	3.98	1.919e-3	3.95	1.162e-05	5.85
0.025	1.333e-4	3.99	1.209e-4	3.99	1.861e-07	5.96
0.0125	8.339e-6	4.00	7.571e-6	4.00	2.926e-09	5.99
0.00625	5.213e-7	4.00	4.734e-7	4.00	4.581e-11	6.00

Consider now the following Hamiltonian system[22]:

$$y' := \begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} \sin(y_2) \\ -\sin(y_1) \end{pmatrix}, \quad y(0) = \begin{pmatrix} 0 \\ \frac{1}{2}\pi \end{pmatrix}, \tag{33}$$

whose Hamiltonian is given by $H(y) = \cos(y_1) + \cos(y_2)$. Again, we found that the value of $e(h)$ essentially depends only on the stepsize h, and not on the number of the mesh points, that is on the width of the interval of integration. The obtained values for this quantity are reported in Table 2, for the same methods previously considered.

Table 2 Numerical results relative to problem (33)

	ETR4		ETR$_2$4		TOM6	
h	$e(h)$	rate	$e(h)$	rate	$e(h)$	rate
0.1	4.153e-6	–	7.557e-6	–	1.598e-08	–
0.05	2.602e-7	4.00	4.729e-7	4.00	3.469e-10	5.53
0.025	1.627e-8	4.00	2.956e-8	4.00	5.884e-12	5.88
0.0125	1.017e-9	4.00	1.848e-9	4.00	9.415e-14	5.97

Finally, we consider the two-body problem[14]

$$y' := \begin{pmatrix} y_1' \\ y_2' \\ y_3' \\ y_4' \end{pmatrix} = \begin{pmatrix} -y_3/\rho \\ -y_4/\rho \\ y_1 \\ y_2 \end{pmatrix}, \quad \rho = (y_3^2 + y_4^2)^{\frac{3}{2}}, \quad t \in [0, 10], \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}. \tag{34}$$

In this case, the angular momentum

$$M(y) = y_2 y_3 - y_1 y_4$$

is preserved, along with the Hamiltonian:

$$H(y) = \frac{1}{2}(y_1^2 + y_2^2) - \frac{1}{\sqrt{y_3^2 + y_4^2}}.$$

The initial value of the angular momentum, $M(y(0)) = 0$, is preserved up to machine precision for all the considered methods. Concerning the Hamiltonian, the computed values for $e(h)$ are reported in Table 3.

Table 3 Numerical results relative to problem (34)

	ETR4		ETR$_2$4		TOM6	
h	$e(h)$	rate	$e(h)$	rate	$e(h)$	rate
0.1	5.271e-5	–	8.505e-5	–	3.800e-06	–
0.05	4.172e-6	3.66	7.088e-6	3.58	1.026e-07	5.21
0.025	2.960e-7	3.82	5.189e-7	3.77	2.166e-09	5.57
0.0125	1.976e-8	3.90	3.525e-8	3.88	3.963e-11	5.77

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