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Long-term stability of multi-value methods for ordinary differential equations

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Abstract Much effort is put into the construction of general linear methods with the aim of achieving an excellent long-time behavior for the integration of Hamiltonian systems. In this article, a backward error analysis is presented, which permits to get sharp estimates for the parasitic solution components and for the error in the Hamiltonian. For carefully constructed methods (symmetric and zero growth parameters) the error in the parasitic components typically grows like $h^{p+4}\exp(h^2Lt)$, where p is the order of the method, and L depends on the problem and on the coefficients of the method. This is confirmed by numerical experiments.

Keywords Multi-value methods · general linear methods · backward error analysis · modulated Fourier expansion · parasitic components · Hamiltonian systems · long-term integration

Mathematics Subject Classification (2000) 65L05 · 65L20 · 65P10

1 Introduction

For the long-time integration of dynamical systems it is important to use suitable numerical methods. It is well-known that symplectic one-step methods have an excellent long-time behavior when applied to Hamiltonian systems, symmetric one-step methods are well suited for reversible integrable systems. Also certain classes of linear multistep methods nearly preserve the energy over long times for second order Hamiltonian systems [11].

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Recently, much effort has been put into the construction of G-symplectic general linear methods with zero growth parameters [4,2,3,8], and it is expected to obtain methods with a long-time behavior that is comparable to symplectic (or symmetric) one-step methods. This article studies long-term error estimates for such multi-value methods. We consider systems of differential equations

$$\dot{y} = f(y), \qquad y(0) = y_0. \tag{1}$$

Multi-value methods consist of a *forward step procedure*

$$Y_{n+1} = V\, Y_n + h\, \Phi(h, Y_n), \tag{2}$$

a *starting procedure*

$$Y_0 = S_h(y_0), \tag{3}$$

and a *finishing procedure*

$$y_n = F_h(Y_n), \tag{4}$$

which permits to extract the numerical approximation from Y_n. If d is the dimension of the differential equation (1) and V is a matrix of dimension $r \times r$ (by abuse of notation we write V in (2) instead of the correct $V \otimes I$, where I is the d-dimensional identity matrix), then the vector Y_n is of dimension rd .

If $r > 1$, the recursion of the forward step procedure has parasitic solutions. The aim of the present article is to study the long-time behavior of these parasitic solutions.

We are mainly interested in stable methods having good conservation properties. We therefore assume that all eigenvalues of V are simple and lie on the unit circle. We denote them by $\zeta_1 = 1, \zeta_2, \ldots, \zeta_r$. We let v_j and v_j^* be right and left eigenvectors ($Vv_j = \zeta_j v_j$ and $v_j^* V = \zeta_j v_j^*$) satisfying $v_j^* v_j = 1$. To relate the forward step procedure (2) to the differential equation (1) we assume the *pre-consistency condition*

$$\Phi(0, Y) = Bf(UY), \qquad Uv_1 = \mathbb{1}, \tag{5}$$

where B is an $r \times s$ matrix, U an $s \times r$ matrix, and $\mathbb{1}$ is the vector with all components equal to 1. Again, by abuse of notation, we avoid the heavy tensor notation and use matrices B and U instead of $B \otimes I$ and $U \otimes I$. For $UY = W = (W_i)_{i=1}^s \in \mathbb{R}^{sd}$ the vector $f(W) \in \mathbb{R}^{sd}$ is defined by $f(W) = (f(W_i))_{i=1}^s$. We assume throughout this article that the forward step method is *consistent*. This means that

$$v_1^* \Phi(0, yv_1) = f(y), \tag{6}$$

and, for pre-consistent methods (5), is equivalent to $v_1^* B \mathbb{1} = 1$.

Backward error analysis is a crucial ingredient for the study of the long-time behavior of numerical integrators, and it has successfully been applied to one-step and linear multistep methods. We extend this tool to multi-value methods in Section 2. In this context we study the effect of symmetry on the modified equations and we discuss the role of growth parameters. Section 3 presents the main results: sharp estimates for the parasitic solution components and a proof of the long-time behavior of multi-value methods, when they are applied to Hamiltonian systems. Numerical experiments are shown in Section 4. They confirm the sharpness of the theoretically obtained error estimates.

2 Backward analysis for multi-value methods

With the aim of separating smooth and parasitic components in the numerical solution $y_n = F_h(Y_n)$, we consider approximations to Y_n of the form

$$\widehat{Y}_n = Y(t_n) + \sum_{j=2}^{r} \zeta_j^n \, Z_j(t_n), \tag{7}$$

where $t_n = nh$, and the coefficient functions $Y(t), Z_j(t)$ are independent of n, but depend smoothly on h. Such expansions have first been considered for the study of the long-time behavior of linear multistep methods [9], see also [11]. There is a striking connection to the technique of modulated Fourier expansions, which is applied to the study of the long-time behavior of analytic and numerical solutions for highly oscillatory problems [12].

2.1 Modified differential equation

We derive a system of modified equations for the smooth functions $Y(t)$ and $Z_j(t)$. These modified equations only depend on the forward step procedure, and are independent of the starting and finishing procedures.

Theorem 1 *Consider a forward step procedure (2) with matrix V having simple eigenvalues of modulus 1. Then there exist h-independent real functions $f_l(y_1)$ and complex functions $g_{kl}(y_1), a_{jl}(y_1)$, and $b_{jkl}(y_1)$, such that for an arbitrarily chosen truncation index N and for every solution $y_k(t), z_{kj}(t)$ of the system $(j,k = 1,\dots,r)$*

$$\begin{aligned}
\dot{y}_1 &= f(y_1) + h\, f_1(y_1) + \ldots + h^{N-1} f_{N-1}(y_1) \\
y_k &= h\, g_{k1}(y_1) + \ldots + h^N g_{k,N}(y_1) \qquad \text{for } \ k > 1 \\
\dot{z}_{jj} &= \big(a_{j0}(y_1) + h\, a_{j1}(y_1) + \ldots + h^{N-1} a_{j,N-1}(y_1)\big) z_{jj} \\
z_{jk} &= \big(h\, b_{jk1}(y_1) + \ldots + h^N b_{j,k,N}(y_1)\big) z_{jj} \qquad \text{for } \ k \neq j
\end{aligned} \tag{8}$$

the approximations (7) with

$$Y(t) = \sum_{k=1}^{r} y_k(t)\, v_k, \qquad Z_j(t) = \sum_{k=1}^{r} z_{kj}(t)\, v_k \tag{9}$$

satisfy (2) with a small defect, i.e.,

$$\widehat{Y}_{n+1} = V\, \widehat{Y}_n + h\, \Phi(h, \widehat{Y}_n) + \mathcal{O}(h^{N+1}) + \mathcal{O}(h\|\mathbf{Z}\|^2)$$

as long as $y_1(t_n)$ remains in a compact set. The constant symbolized by $\mathcal{O}(\cdot)$ is independent of h, but depends on the truncation index N. We use the notation $\|\mathbf{Z}\| = \max\{|z_{jk}(t_n)|\,;\, j,k = 1,\dots,r\}$.

Proof Inserting (7) into the forward step procedure and expanding the nonlinearity around $Y(t_n)$ yields

$$\begin{aligned} Y(t+h) &= V\,Y(t) + h\,\Phi\big(h, Y(t)\big) + \mathcal{O}(h\|\mathbf{Z}\|^2) \\ \zeta_j\,Z_j(t+h) &= V\,Z_j(t) + h\,\Phi'\big(h, Y(t)\big)\,Z_j(t) + \mathcal{O}(h\|\mathbf{Z}\|^2). \end{aligned} \tag{10}$$

Neglecting terms of size $\mathcal{O}(h\|\mathbf{Z}\|^2)$ and using (9), we get from the upper relation

$$y_k(t+h) = \zeta_k y_k(t) + h\,v_k^*\Phi\big(h, Y(t)\big).$$

We expand the left-hand side into a Taylor series around $h=0$ and thus obtain (omitting the argument t)

$$\begin{aligned} \dot y_1 + \frac{h}{2}\,\ddot y_1 + \cdots &= \Psi_1(h, y_1, \ldots, y_r) \\ (1-\zeta_k)\,y_k + h\,\dot y_k + \frac{h^2}{2}\,\ddot y_k + \cdots &= h\Psi_k(h, y_1, \ldots, y_r), \quad k = 2, \ldots, r. \end{aligned} \tag{11}$$

Differentiation of the relations for y_k $(k=2,\ldots,r)$ and recursive elimination of the first and higher derivatives, and also of $y_2, \ldots, y_r$ on the right-hand side, yields the second relation of (8) with a defect of size $\mathcal{O}(h^{N+1})$. In the same way one can eliminate the second and higher derivatives in the first equation of (11) and thus obtains a differential equation for y_1. By the consistency assumption (6), the h-independent term of this differential equation becomes $f(y_1)$.

Neglecting terms of size $\mathcal{O}(h\|\mathbf{Z}\|^2)$ in the second relation of (10) yields

$$\zeta_j z_{kj}(t+h) = \zeta_k z_{kj}(t) + h\,v_k^*\Phi'\big(h, Y(t)\big)\,Z_j(t). \tag{12}$$

We expand the left-hand side into a Taylor series, and apply the same elimination procedure as for the smooth component $Y(t)$. This then gives a first order differential equation for z_{jj} and algebraic relations for z_{kj} $(k \neq j)$, and terminates the proof of (8). □

2.2 Initial values

For $n=0$ and $\widehat{Y}_0 = Y_0 = S_h(y_0)$ the relation (7) gives

$$S_h(y_0) = Y(0) + \sum_{j=2}^{r} Z_j(0).$$

Because of the algebraic relations in (8) this represents a nonlinear algebraic equation for the h-dependent vectors $y_1(0), z_{22}(0), \ldots, z_{rr}(0)$. For $h=0$ we get

$$y_1(0)\big|_{h=0} = v_1^* S_0(y_0), \qquad z_{jj}(0)\big|_{h=0} = v_j^* S_0(y_0),$$

and the implicit function theorem guarantees the existence of a local unique solution for sufficiently small h.

The initial values $z_{jj}(0)$ for $j = 2, \dots, r$ determine, on intervals of length $\mathcal{O}(1)$, the size of the parasitic solution components. We shall investigate how they depend on the choice of the starting procedure. Let us denote the forward step procedure (2) by $Y_{n+1} = G_h(Y_n)$. It follows from Theorem XV.8.2 of [13] that for a given $G_h(Y)$ and a given finishing procedure $F_h(Y)$ there exist a unique (as formal power series in h) starting procedure $S_h^*(y)$ and a unique one-step method $y_{n+1} = \Phi_h^*(y_n)$, such that

$$G_h \circ S_h^* = S_h^* \circ \Phi_h^* \qquad \text{and} \qquad F_h \circ S_h^* = \text{identity}. \tag{13}$$

This means that for the choice $Y_0 = S_h^*(y_0)$ the numerical solution obtained by the multi-value method is (formally) equal to that of the one-step method Φ_h^*. For this reason, the method Φ_h^* is called *underlying one-step method*.

For all common multi-value methods and in particular for general linear methods (see [1]) the underlying one-step method and the components of the starting procedure are B-series. Their coefficients can be computed recursively from the relations (13) by using the composition formula for B-series.

Theorem 2 *Let the starting procedure $S_h(y_0)$ satisfy*

$$S_h(y_0) = S_h^*(y_0) + \mathcal{O}(h^q), \tag{14}$$

and assume that the finishing procedure is given by $F_h(Y) = v_1^* Y = y_1$. Then, the initial values for the system of modified equations (8) satisfy

$$y_1(0) = y_0 + \mathcal{O}(h^q), \qquad z_{jj}(0) = \mathcal{O}(h^q).$$

Proof For the exact starting procedure $S_h^*(y_0)$ the numerical solution $\{y_n\}_{n\geq 0}$ is that of the underlying one-step method and does not have parasitic components. Consequently, we have $y_1(0) = y_0$ and $z_{kj}(0) = 0$ for all k and j. A perturbation of this starting procedure implies, by the implicit function theorem, a perturbation of the same size in the initial values $y_1(0), z_{22}(0), \dots, z_{rr}(0)$. □

Remark 1 For a finishing procedure, given by $F_h(Y) = v_1^* Y$ (which is the typical situation), the numerical solution is close to $y_n = y_1(t_n) + \sum_{j=2}^{r} \zeta_j^n z_{1j}(t_n)$, and the modified differential equation of the underlying one-step method is the differential equation of (8) for y_1. If this one-step method is of order p, then we have $f_j(y_1) = 0$ for $j = 1, \dots, p-1$ in the modified equation.

If $F_h(Y) = d^{\mathsf{T}} Y + \mathcal{O}(h)$ with $d^{\mathsf{T}} v_1 = 1$ then, due to the algebraic relations (8) for $y_k, k = 2, \dots, r$, there is a bijection $F_h(Y) \leftrightarrow v_1^* Y = y_1$ which permits to obtain the modified equation for the underlying one-step method from (8).

2.3 Growth parameters

The parasitic solution components are determined by the functions $z_{jj}(t)$. To study their long-time behavior we first examine the leading term in the differential equation (8) for z_{jj}. For $k = j$ the equation (12) yields

$$\zeta_j \, \dot{z}_{jj} = v_j^* \Phi'(0, y_1 v_1) \, v_j z_{jj} + \mathcal{O}(h|z_{jj}|).$$

Subject to the pre-consistency assumption (5), we obtain

$$\dot{z}_{jj} = \mu_j \, f'(y_1) \, z_{jj} + \mathcal{O}(h|z_{jj}|), \qquad \mu_j = \zeta_j^{-1} \, v_j^* B U v_j. \tag{15}$$

The coefficients μ_j are called *growth parameters* of the multi-value method. They determine to a large extent the long-term behavior of the parasitic components $Z_j(t)$. For linear multistep methods with generating polynomials (ρ, σ) these growth parameters, given by $\mu_j = \sigma(\zeta_j)/(\zeta_j \rho'(\zeta))$ and introduced in [6], cannot be zero for irreducible methods.

However, recently, general linear methods have been constructed [4] for which the growth parameters corresponding to parasitic roots are all zero. This is an interesting property in view of the long-term energy conservation in the numerical solution of Hamiltonian differential equations.

2.4 Modified differential equation of symmetric methods

Consider a multi-value method, equipped with a finishing procedure. We call it *symmetric* (see [13]) if the underlying one-step method is symmetric, i.e., if $\Phi_h^* = (\Phi_{-h}^*)^{-1}$. This implies that the modified differential equation of Φ_h^* is in even powers of h. Without additional assumptions on the method, we cannot expect to have a similar result for the whole system (8).

Theorem 3 *Consider a forward step procedure (2), where V is of dimension 2 with eigenvalues 1 and -1, and assume that it is mathematically equivalent to*

$$Y_n = V \, Y_{n+1} - h \, \Phi(-h, Y_{n+1}).$$

Then, the equations (8) of Theorem 1 contain only expressions with even powers of h.

Proof Neglecting terms of size $\mathcal{O}(h^{N+1})$ and $\mathcal{O}(h\|\mathbf{Z}\|^2)$, the functions $Y(t)$ and $Z_j(t)$ of Theorem 1 satisfy

$$\begin{aligned} Y(t+h) &= V \, Y(t) + h \, \Phi\big(h, Y(t)\big) \\ \zeta_j \, Z_j(t+h) &= V \, Z_j(t) + h \, \Phi'\big(h, Y(t)\big) \, Z_j(t), \end{aligned} \tag{16}$$

where the prime in $\Phi'(h, Y)$ stands for a derivative with respect to Y. Our assumption on the forward step procedure implies that

$$\begin{aligned} Y(t) &= V \, Y(t+h) - h \, \Phi\big(-h, Y(t+h)\big) \\ Z_j(t) &= V \, \zeta_j \, Z_j(t+h) - h \, \Phi'\big(-h, Y(t+h)\big) \, \zeta_j \, Z_j(t+h), \end{aligned}$$

which, substituting $t-h$ for t, gives

$$\begin{aligned} Y(t-h) &= V\,Y(t) - h\,\Phi\big(-h, Y(t)\big) \\ \zeta_j^{-1} Z_j(t-h) &= V\,Z_j(t) - h\,\Phi'\big(-h, Y(t)\big)\,Z_j(t), \end{aligned} \tag{17}$$

Let us consider first the components of the vector $Y(t)$. Comparing the upper relations of (16) and (17) we notice that the components $y_k(t)$ of $Y(t)$ have to satisfy the same equations for h and for $-h$.

Since, by assumption, $\zeta_2 = -1$ is the only eigenvalue of V different from 1, we have $\zeta_2^{-1} = \zeta_2$. The lower relation of (16) is therefore equal to the lower relation of (17), where h is replaced by $-h$. Consequently, also the components of $Z_2(t)$ have to satisfy the same equations for h and for $-h$. This implies that all equations of (8) are in even powers of h. □

3 Long-term behavior of multi-value methods

Insight into the long-term behavior of multi-value methods requires

- the study of properties of the underlying one-step method. Its modified differential equation is closely related to the equation for y_1 in (8).
- the study of boundedness of the parasitic solution components, which are given by the differential and algebraic equations for z_{jk} in (8).

3.1 Bounds on the parasitic solution components

It follows from Theorem 1 that the coefficient functions of the parasitic solution components (9) satisfy

$$\begin{aligned} \dot{z}_{jj} &= h^M A\big(h, y_1(t)\big)\, z_{jj} \\ z_{jk} &= h\,B\big(h, y_1(t)\big)\, z_{jj} \qquad \text{for } k \neq j. \end{aligned} \tag{18}$$

In general we have $M = 0$, but if the growth parameters (15) of the method are zero we have $M = 1$, and if in addition to zero growth parameters the assumptions of Theorem 3 are satisfied we have $M = 2$. If the vector field $f(y)$ of (1) is smooth and has bounded derivatives (which excludes stiff and highly oscillatory problems), the functions $A(h, y_1)$ and $B(h, y_1)$ are bounded as long as $y_1(t)$ stays in a compact set. Gronwall's Lemma then implies

$$\|z_{jj}(t)\| \leq \|z_{jj}(0)\| \exp(h^M L t), \tag{19}$$

where L is a bound on the norm or, better, the logarithmic norm of $A(h, y_1)$. For $k \neq j$ the functions $z_{jk}(t)$ are bounded by the same expression with an additional factor Ch.

3.2 Energy conservation for Hamiltonian systems

For a Hamiltonian system

$$\dot{y} = J^{-1}\nabla H(y), \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{20}$$

the Hamiltonian function $H(y)$, also called energy, is preserved along exact solutions. We are interested to know how well the energy is preserved by the numerical solution of a multi-value method.

Theorem 4 *Consider a multi-value method of order p, a starting procedure satisfying (14) with q, and let $0 \le M \le q$ be the integer such that the modified equations for z_{jj}, $j = 2, \dots, r$, satisfy (18). Furthermore, assume the existence of a modified Hamiltonian $\widetilde{H}(y)$ satisfying $\widetilde{H}(y) - H(y) = \mathcal{O}(h^p)$ which is well preserved by the flow $\widetilde{\varphi}_t(y)$ of the underlying one-step method, more precisely,*

$$\widetilde{H}\big(\widetilde{\varphi}_h(y)\big) = \widetilde{H}(y) + \mathcal{O}(h^{r+1}) \tag{21}$$

with $p \le r \le 2q$. We then have, for $t = nh$,

$$H(y_n) - H(y_0) = \mathcal{O}(h^p) + \mathcal{O}(th^r) + \mathcal{O}\big(h^{q+1}\exp(h^M L t)\big)$$

as long as $t = \mathcal{O}(h^{-M})$.

Proof Recall that for a given initial value y_0 the numerical solution is obtained from $Y_0 = S_h(y_0)$, the forward step procedure $Y_{n+1} = VY_n + h\Phi(h, Y_n)$, and the finishing procedure $y_n = F_h(Y_n)$. The proof is in several steps.

a) We use the expansion (7) only locally on one step. This means that for every n we compute functions $Y^{[n]}(t)$ and $Z_j^{[n]}(t)$ satisfying the modified equations (8) such that

$$Y_n = Y^{[n]}(0) + \sum_{j=2}^{r} Z_j^{[n]}(0).$$

It follows from Theorem 1 that (with the choice $N = 2q$)

$$Y_{n+1} = Y^{[n]}(h) + \sum_{j=2}^{r} \zeta_j Z_j^{[n]}(h) + \mathcal{O}(h^{2q+1})$$

as long as the parasitic components are bounded as $\|Z(t)\| = \mathcal{O}(h^q)$. By the uniqueness of the initial values (Section 2.2) this implies that

$$Y^{[n+1]}(0) = Y^{[n]}(h) + \mathcal{O}(h^{2q+1}), \qquad Z_j^{[n+1]}(0) = \zeta_j Z_j^{[n]}(h) + \mathcal{O}(h^{2q+1}). \tag{22}$$

b) The estimates (19) and (22) yield

$$\|z_{jj}^{[n+1]}(0)\| \le \|z_{jj}^{[n]}(h)\| + Ch^{2q+1} \le \|z_{jj}^{[n]}(0)\|\exp(h^{M+1}L) + Ch^{2q+1}.$$

Applying a discrete Gronwall Lemma we obtain for $t = nh$

$$\|z_{jj}^{[n]}(0)\| \le \|z_{jj}^{[0]}(0)\| \exp(h^M L t) + C h^{2q}\, t\, \exp(h^M L t). \tag{23}$$

c) We assume now that the finishing procedure is given by $F_h(Y) = v_1^* Y$, so that the time-h flow of the modified equation for y_1 in (8) represents the underlying one-step method. (For a more general finishing procedure, the nonlinear transformation of Remark 1 has to be considered.) We consider the telescoping sum

$$\widetilde{H}\big(y_1^{[n]}(0)\big) - \widetilde{H}\big(y_1^{[0]}(0)\big) = \sum_{l=0}^{n-1} \Big(\widetilde{H}\big(y_1^{[l+1]}(0)\big) - \widetilde{H}\big(y_1^{[l]}(0)\big) \Big).$$

From the estimate (22) and the assumption (21) we obtain that every summand is bounded by $\mathcal{O}(h^{2q+1}) + \mathcal{O}(h^{r+1})$ (the first term can be removed, because $r \le 2q$), which yields an error term of size $\mathcal{O}(th^r)$. In the left-hand side we substitute $y_1^{[n]}(0)$ from the relation

$$y_n = y_1^{[n]}(0) + \sum_{j=2}^{r} z_{1j}^{[n]}(0). \tag{24}$$

The statement now follows from $\|z_{1j}(0)\| \le ch\|z_{jj}(0)\|$, from the bounds (23) for $z_{jj}^{[n]}(0)$, and from the assumption $\widetilde{H}(y) - H(y) = \mathcal{O}(h^p)$. □

Similar long-time behavior (with terms increasing exponentially like $\exp(h^M L t)$) has been obtained in [5] for partitioned linear multistep methods. It is interesting that certain linear multistep methods for second order differential equations have an excellent energy preservation without any exponential terms [11].

The crucial ingredient of the previous theorem is the existence of a modified Hamiltonian function. Let us discuss the most important situations where such a modified Hamiltonian is known to exist.

- If the underlying one-step method is a symplectic transformation, there exists a modified Hamiltonian satisfying (21) with arbitrarily large r, see [13, Section IX.3]. Unfortunately, the results of [10] indicate that the underlying one-step method of multi-value methods cannot be symplectic.
- If (20) is an integrable reversible system, and if the underlying one-step method is symmetric (reversible), under mild non-resonance conditions there exists a modified Hamiltonian satisfying (21) with arbitrarily large r, see [13, Chapter XI].
- If the underlying one-step method is a B-series (this is the case for all general linear methods), necessary and sufficient conditions for the existence of a modified Hamiltonian satisfying (21) with a given r are presented in [13, IX.9.4]. For example, only one condition is necessary for symmetric methods of order 4 to satisfy condition (21) with $r = 6$.

– If the underlying one-step method is a B-series, necessary and sufficient conditions for conjugate-symplecticity up to a certain order r are given in [15]. This implies the existence of $\widetilde{H}(y)$ satisfying (21). For example, three conditions are necessary for methods of order 4 to satisfy condition (21) with $r = 5$.

Remark 2 A recent result of [7] shows that G-symplecticity of a general linear method implies conjugate-symplecticity of the underlying one-step method. Consequently, the assumption (21) is satisfied with arbitrarily large r, and the second (linearly increasing) term in the estimate of Theorem 4 can be removed.

The factor h^q in front of the exponentially increasing term can be made smaller by designing starting procedures that better approximate $S_h^*(y)$. To get results on intervals longer than $\mathcal{O}(h^{-2})$, one has either to construct methods for which also the h^2-term in the modified differential equation for $z_{jj}(t)$ vanishes or one has to restrict the class of methods and the class of problems that permit to get improved bounds on $z_{jj}(t)$.

3.3 Further results on the long-time behavior

The estimates (19) prove that for multi-value methods for which the order q of the starting procedure is larger or equal to the order p of the method, the parasitic solution components can be neglected on time intervals of length $\mathcal{O}(h^{-M})$. On such intervals the underlying one-step method completely describes the qualitative behavior of the method and we have the following results:

– If the problem is an integrable reversible system and if the underlying one-step method is symmetric (and reversible), then all action variables are preserved up to an error of size $\mathcal{O}(h^p)$. Moreover, the global error increases at most linearly with time.
– If the underlying one-step method is conjugate-symplectic up to order $r > p$, then quadratic first integrals (like the angular momentum) are conserved up to an error of size $\mathcal{O}(h^p) + \mathcal{O}(th^r)$. The same estimates hold for action variables in integrable Hamiltonian systems.

4 Application to general linear methods

The aim of this section is to illustrate with numerical experiments that the bounds of Theorem 4 and, in particular, those for the parasitic solution components are sharp. We consider general linear methods, which are given by the formulas (with the notation of Section 1)

$$Y_{n+1} = VY_n + hBf(W), \qquad W = UY_n + hAf(W).$$

4.1 A general linear method with zero growth parameters

The general linear method with coefficients

$$\left|\begin{array}{cc|cccc} 1 & 0 & 2/3 & -1/6 & -1/6 & 2/3 \\ 0 & -1 & 1 & -1/2 & 1/2 & -1 \\ \hline 1 & 1/2 & 1/12 & 0 & 0 & 0 \\ 1 & 1 & -1/3 & 1/6 & 0 & 0 \\ 1 & -1 & 5/3 & -2/3 & 1/6 & 0 \\ 1 & -1/2 & 7/6 & -5/12 & 1/12 & 1/12 \end{array}\right|$$

(the matrices V and B are in the upper row, and U and A in the lower row) has recently been proposed in [4]. We have 2 external stages and 4 internal stages, and the matrix V has eigenvalues $\zeta_1 = 1$ and $\zeta_2 = -1$. The vector

$$Y_n = \begin{pmatrix} y_n \\ a_n \end{pmatrix}$$

provides an approximation y_n to the solution and an approximation a_n to a scaled second derivative. The finishing procedure is the mapping $F_h(Y_n) = y_n$. If we denote by $R_h(y_0)$ the result of one step of the Runge–Kutta method

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1 & 373/550 & 177/550 & & \\ 0 & 8233/50976 & -30749/152928 & 3025/76464 & \\ \hline & 0 & -383/648 & 275/1296 & 1 \end{array}$$

then the starting procedure is given by

$$S_h(y_0) = \begin{pmatrix} y_0 \\ \frac{1}{2}\big(R_h(y_0) + R_{-h}(y_0)\big) - y_0 \end{pmatrix}.$$

Let us collect some essential properties of this method.

- The method is of order $p = 4$ implying that the underlying one-step method is of order 4.
- The method is symmetric in the sense of Theorem 3. As a consequence all equations in (8) are in even powers of h.
- By construction, the growth parameter corresponding to the parasitic root $\zeta_2 = -1$ is zero. Together with the symmetry of the method this implies that $M = 2$ in (18).
- The first component of the exact starting procedure $S_h^*(y)$ is the identity (as it is the case for $S_h(y)$). The B-series of the second component of $S_h^*(y)$, computed from the relations (13), has coefficients[1]

$\emptyset$	$\bullet$	$[\bullet]$	$[\bullet,\bullet]$	$[[\bullet]]$	$[\bullet,\bullet,\bullet]$	$[\bullet,[\bullet]]$	$[[\bullet,\bullet]]$	$[[[\bullet]]]$
0	0	$-1/12$	0	0	239/10368	59/1728	11/3456	11/1728

[1] All the manipulations with B-series are done with the excellent Mathematica package by Ander Murua.

with zero coefficients for trees with odd order. Computing the B-series of the starting procedure $S_h(y)$, we find that $S_h(y) = S_h^*(y) + \mathcal{O}(h^6)$, so that $q = 6$.

– We have computed the dominant error term of the underlying one-step method. The coefficients for the trees of order 5 are

$[\bullet,\bullet,\bullet,\bullet]$	$[\bullet,\bullet,[\bullet]]$	$[\bullet,[\bullet,\bullet]]$	$[\bullet,[[\bullet]]]$	$[[\bullet],[\bullet]]$
839/124416	491/10368	349/10368	169/5184	251/10368

$[[\bullet,\bullet,\bullet]]$	$[[\bullet,[\bullet]]]$	$[[[\bullet,\bullet]]]$	$[[[[\bullet]]]]$
457/31104	157/5184	83/10368	47/5184

Verifying the conditions of Theorem VI.8.3 of [13] we find that the method is conjugate-symplectic up to order at least 5. Since the method is symmetric, it is automatically conjugate-symplectic up to order 6. Checking the criterion of [15] we have even found that the underlying one-step method is conjugate-symplectic up to order 8, so that (21) is satisfied with $r = 8$, see also [7].

Theorem 5 *If the method of this section is applied to a Hamiltonian system (20), then the energy is nearly preserved according to*

$$H(y_n) - H(y_0) = \mathcal{O}(h^4) + \mathcal{O}(th^8) + \mathcal{O}\big(h^8 \exp(h^2 L t)\big)$$

as long as $t = nh = \mathcal{O}(h^{-2})$.

Proof The first two error terms follow directly from Theorem 4. From Theorem 2 we have that the parasitic solution components satisfy $z_{jj}(0) = \mathcal{O}(h^6)$, so that $z_{jj}(t) = \mathcal{O}\big(h^6 \exp(h^2 L t)\big)$. To justify the factor h^8 in front of the exponential term we note that only the functions z_{1j} enter the formula for y_n. By symmetry of the method, we have a factor h^2 in the modified equation (8) for z_{1j}. This proves that $z_{1j}(t) = \mathcal{O}\big(h^8 \exp(h^2 L t)\big)$. □

4.2 Numerical experiments

To prove that the estimate of Theorem 5 is sharp, we apply the method of Section 4.1 to the mathematical pendulum with the Hamiltonian

$$H(p,q) = \frac{1}{2}\, p^2 - \cos q,$$

and initial values $q(0) = 3$, $p(0) = 0$ as in [4]. We use constant step sizes. Figure 2 shows the error in the Hamiltonian as a function of time for the step sizes $h = 0.25$ and $h = 0.125$. The scales on the vertical axis differ by a factor 16, so that the $\mathcal{O}(h^4)$ behavior of the error can be observed. As predicted by the estimate of Theorem 5 the error behaves like $\mathcal{O}(h^4)$ on intervals of length $\mathcal{O}(h^{-2})$, and then follows an exponential growth. We notice that halving the step size increases the interval of good energy preservation by a factor of 4. This confirms the factor h^2 in the exponential term. The constant L in the estimate, which depends on the problem and on the coefficients of the method, seems to be rather small.

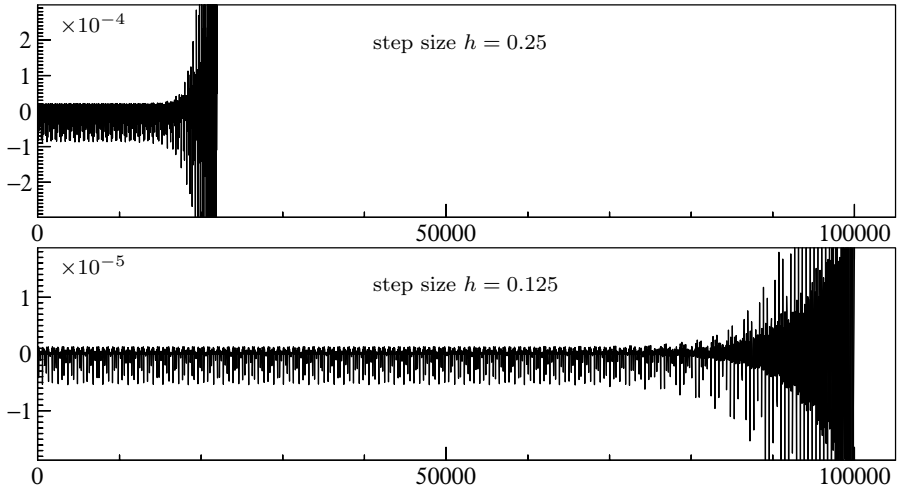

Fig. 1 Error in the Hamiltonian for the method of Section 4.1 applied to the mathematical pendulum with initial values $q(0) = 3$, $p(0) = 0$.

4.3 Methods with complex parasitic roots

For general linear methods with a matrix V having complex eigenvalues, we cannot apply Theorem 3. Let us compute the dominant terms in the modified equations of Theorem 1 following its constructive proof. For $k > 1$, we obtain

$$y_k = h\nu_{k1} f(y_1) + h^2 \nu_{k2} f'(y_1) f(y_1) + \mathcal{O}(h^3),$$

where $\nu_{k1} = (1 - \zeta_k)^{-1} v_k^* B \mathbb{1}$. If the coefficients ν_{k1} vanish for all $k > 1$, then we have $\nu_{k2} = (1 - \zeta_k)^{-1} v_k^* BA\mathbb{1}$.

The differential equation for z_{jj} has the form

$$\dot{z}_{jj} = \Big(\mu_j f'(y_1) + h\Big(\mu_{j1} f'(y_1) f'(y_1) + \mu_{j2} f''(y_1)\big(f(y_1), \cdot\big)\Big) + \mathcal{O}(h^2) \Big) z_{jj},$$

where $\mu_j = \zeta_j^{-1} v_j^* BU v_j$ is the growth paremeter associated to ζ_j, and the further coefficients are given by

$$\mu_{j1} = \frac{v_j^* BAU v_j}{\zeta_j} + \sum_{k \neq j, k \neq 1} \frac{v_j^* BU v_k v_k^* BU v_j}{\zeta_j(\zeta_j - \zeta_k)} - \frac{\mu_j^2}{2}$$

$$\mu_{j2} = \frac{v_j^* B(c \cdot U v_j)}{\zeta_j} - \frac{\mu_j}{2}, \qquad c = A\mathbb{1} + \sum_{k=2}^{r} \nu_{k1}\, U v_k.$$

We now consider the method 4134 of [4] with coefficients given by

$$\left|\begin{array}{ccc|ccc|c} 1 & 0 & 0 & -1/10 & 3/5 & 3/5 & -1/10 \\ 0 & 0 & 1 & -1/5 & 6/5 & -6/5 & 1/5 \\ 0 & -1 & 0 & \sqrt{5}/5 & 0 & 0 & -\sqrt{5}/5 \\ \hline 1 & -\sqrt{5}/12 & -1/12 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1/12 & -1/12 & 1/4 & 0 & 0 \\ 1 & 0 & 1/12 & -7/60 & 7/10 & 1/4 & 0 \\ 1 & \sqrt{5}/12 & 1/12 & -1/5 & 7/10 & 1/2 & 0 \end{array}\right| .$$

For this method, whose matrix V has eigenvalues 1, i, and $-$i and which has zero growth parameters μ_j, it turns out that $\nu_{k1} = 0$, $\nu_{k2} \neq 0$ for all k, and $\mu_{j1} = \mu_{j2} = 0$ for all j. Similar as in the previous example the parasitic solution components are bounded by $h^r \exp(h^2 L t)$, where r depends on the accuracy of the starting procedure.

To verify our estimates also in the case of complex parasitic roots, we have constructed a starting procedure satisfying (14) with $q = 5$. It is given by

$$S_h(y_0) = \begin{pmatrix} y_0 \\ R_h^2(y_0) - y_0 \\ R_h^3(y_0) - y_0 \end{pmatrix},$$

where $R_h^2(y_0)$ and $R_h^3(y_0)$ are explicit Runge–Kutta methods with 4 stages. For the finishing procedure, which consists of taking the first component as numerical approximation, we computed the B-sries of the corresponding exact starting procedure $S_h^*(y_0)$. Their coefficients up to order four are given in Table 1. The order conditions for the methods $R_h^2(y_0)$ and $R_h^3(y_0)$ are those for explicit Runge–Kutta methods (see for example [14, pages 135–136]), where the fraction of the right-hand side is replaced by the coefficients of Table 1.

We arbitrarily fix $c_3 = 1/2$ and $c_4 = 1$, and we consider c_2 as a parameter. The coefficients a_{ij} and b_j can then be computed straightforwardly following the construction of explicit Runge–Kutta methods of order 4 with 4 stages.

Table 1 Coefficients of the B-series for the exact starting procedure of method 4134

tree	method $R_h^2(y_0)$	method $R_h^3(y_0)$
$\bullet$	0	0
$[\bullet]$	$\frac{3-\sqrt{5}}{10}$	$\frac{-3-\sqrt{5}}{10}$
$[\bullet,\bullet]$	$\frac{-3-\sqrt{5}}{10}$	$\frac{-3+\sqrt{5}}{10}$
$[[\bullet]]$	$\frac{-35-16\sqrt{5}}{300}$	$\frac{-35+16\sqrt{5}}{300}$
$[\bullet,\bullet,\bullet]$	$\frac{-59+18\sqrt{5}}{90}$	$\frac{59+18\sqrt{5}}{90}$
$[\bullet,[\bullet]]$	$\frac{-187+60\sqrt{5}}{600}$	$\frac{187+60\sqrt{5}}{600}$
$[[\bullet,\bullet]]$	$\frac{-135+38\sqrt{5}}{600}$	$\frac{135+38\sqrt{5}}{600}$
$[[[\bullet]]]$	$\frac{-131+37\sqrt{5}}{1200}$	$\frac{131+37\sqrt{5}}{1200}$

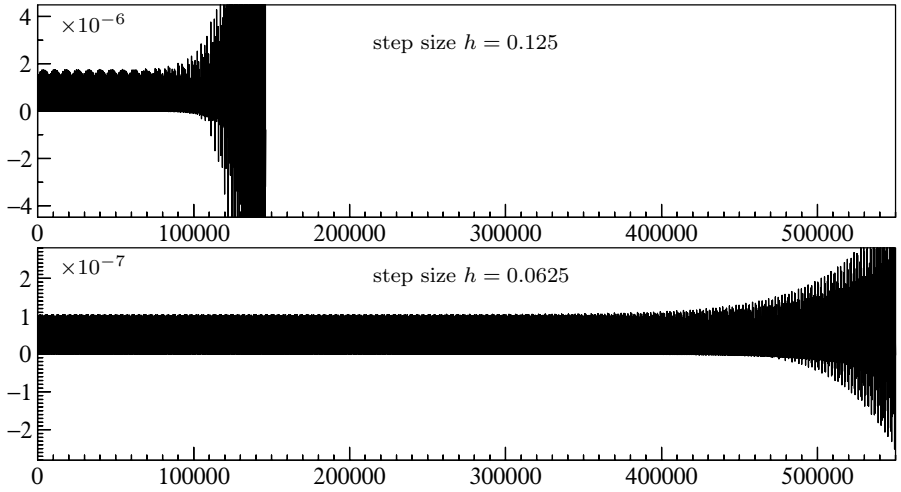

Fig. 2 Error in the Hamiltonian for the method of Section 4.3 applied to the mathematical pendulum with initial values $q(0) = 3$, $p(0) = 0$.

The last order condition leads to a polynomial equation of degree 3 for the parameter c_2 with real solution

$$c_2 = \frac{20429509 + 5835398\sqrt{5}}{177874806} \qquad \text{and} \qquad c_2 = \frac{-17237489 + 7047906\sqrt{5}}{248413686}$$

for the methods $R_h^2(y_0)$ and $R_h^3(y_0)$, respectively.

We have applied the method 4134 with our starting procedure to the mathematical pendulum with data as in Figure 2. Similar to the method of Section 4.1 we can observe an exponential growth of the parasitic solution components. For the step size $h = 0.125$ it becomes clearly visible after $t = 90\,000$, and for $h = 0.0625$ after $t = 400\,000$. This agrees very well with our theoretical estimates.

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