Long-Term Stability of Symmetric Partitioned Linear Multistep Methods

Paola Console and Ernst Hairer

Abstract Long-time integration of Hamiltonian systems is an important issue in many applications – for example the planetary motion in astronomy or simulations in molecular dynamics. Symplectic and symmetric one-step methods are known to have favorable numerical features like near energy preservation over long times and at most linear error growth for nearly integrable systems. This work studies the suitability of linear multistep methods for this kind of problems. It turns out that the symmetry of the method is essential for good conservation properties, and the more general class of partitioned linear multistep methods permits to obtain more favorable long-term stability of the integration. Insight into the long-time behavior is obtained by a backward error analysis, where the underlying one-step method and also parasitic solution components are investigated. In this way one approaches a classification of problems, for which multistep methods are an interesting class of integrators when long-time integration is important. Numerical experiments confirm the theoretical findings.

1 Introduction

Linear multistep methods are an important alternative to Runge–Kutta one-step methods for the numerical solution of ordinary differential equations. Adams-type methods are frequently used for the integration of nonstiff differential equations, and BDF schemes have excellent properties for the solution of stiff differential equations. In the context of 'geometric numerical integration', where structure-preservation and long-time integration are important, there has been a remarkable

Paola Console
Section de Mathématiques, Université de Genève, e-mail: Paola.Console@unige.ch

Ernst Hairer
Section de Mathématiques, Université de Genève, e-mail: Ernst.Hairer@unige.ch

publication [15], where certain symmetric multistep methods for second order differential equations have been successfully applied to the integration of planetary motion. A theoretical explanation of the observed excellent long-time behavior has been given in [9]. It is based on a backward error analysis, and rigorous estimates for the parasitic solution components are obtained, when the system is Hamiltonian of the form $\ddot{q} = -\nabla U(q)$, and derivative approximations are obtained locally by finite differences.

The main aim of the present contribution is to study to which extend this excellent behavior and its theoretical explanation is valid also in more general situations – separable Hamiltonians $H(p,q) = T(p) + U(q)$ with general functions $T(p)$ and $U(q)$, and problems with position dependent kinetic energy. The presentation of the results is in three parts. In the first part we briefly recall the classical theory of partitioned linear multistep methods (order, zero-stability, convergence) and known results on the long-time behavior of symmetric multistep methods for second order Hamiltonian systems. We also present numerical experiments illustrating an excellent long-time behavior in interesting situations. The theoretical explanation of the long-time behavior is based on a backward error analysis for partitioned multistep methods. Part 2 is devoted to the study of the underlying one-step method. This method is symmetric, and we investigate conditions on the coefficients of the method to achieve good conservation of the Hamiltonian. When using multistep methods one is necessarily confronted with parasitic solution components, because the order of the difference equation is higher than the order of the differential equation. These parasitic terms will be studied in Part 3. On time intervals, where the parasitic terms remain bounded and small, the multistep method essentially behaves like a symmetric one-step method.

1.1 Classical Theory of Partitioned Linear Multistep Methods

Hamiltonian systems are partitioned ordinary differential equations of the form

$$\begin{aligned} \dot{p} &= f(p,q), \quad p(0) = p_0, \\ \dot{q} &= g(p,q), \quad q(0) = q_0, \end{aligned} \tag{1}$$

where $f(p,q) = -\nabla_q H(p,q)$, $g(p,q) = \nabla_p H(p,q)$, and $H(p,q)$ is a smooth scalar energy function. For their numerical solution we consider partitioned linear multistep methods

$$\begin{aligned} \sum_{j=0}^{k} \alpha_j^p p_{n+j} &= h \sum_{j=0}^{k} \beta_j^p f(p_{n+j}, q_{n+j}) \\ \sum_{j=0}^{k} \alpha_j^q q_{n+j} &= h \sum_{j=0}^{k} \beta_j^q g(p_{n+j}, q_{n+j}), \end{aligned} \tag{2}$$

where the p and q components are discretized by different multistep methods. Following the seminal thesis of Dahlquist, we denote the generating polynomials of the

coefficients α_j, β_j of a multistep method by

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \qquad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j.$$

The generating polynomials of the method (2) are thus $\rho_p(\zeta)$, $\sigma_p(\zeta)$ and $\rho_q(\zeta)$, $\sigma_q(\zeta)$, respectively. In the following we collect some basic properties of linear multistep methods (see e.g., [12]).

Zero-stability. A linear multistep method is called stable, if the polynomial $\rho(\zeta)$ satisfies the so-called *root condition*, i.e., all zeros of the equation $\rho(\zeta) = 0$ satisfy $|\zeta| \le 1$, and those on the unit circle are simple.

Order of consistency. A linear multistep method has order r if

$$\frac{\rho(\zeta)}{\log \zeta} - \sigma(\zeta) = \mathscr{O}\big((\zeta - 1)^r\big) \quad \text{for} \quad \zeta \to 1.$$

For a given polynomial $\rho(\zeta)$ of degree k satisfying $\rho(1) = 0$, there exists a unique $\sigma(\zeta)$ of degree k such that the order of the method is at least $k+1$; and there exists a unique $\sigma(\zeta)$ of degree $k-1$ (which yields an explicit method) such that the order of the method is at least k.

Convergence. If both methods of (2) are stable and of order r, then we have convergence of order r. This means that for sufficiently accurate starting approximations and for $t_n = nh \le T$ we have

$$\|p_n - p(t_n)\| + \|q_n - q(t_n)\| \le C(T)\, h^r \quad \text{for} \quad h \to 0. \tag{3}$$

The constant $C(T)$ is independent of n and h. It typically increases exponentially as a function of T.

Symmetry. A multistep method is symmetric if the coefficients satisfy $\alpha_j = -\alpha_{k-j}$ and $\beta_j = \beta_{k-j}$ for all j. In terms of the generating polynomials this reads

$$\rho(\zeta) = -\zeta^k \rho(1/\zeta), \qquad \sigma(\zeta) = \zeta^k \sigma(1/\zeta). \tag{4}$$

If $\alpha_0 = 0$, the number k has to be reduced in this definition. Symmetry together with zero-stabilty imply that all zeros of $\rho(\zeta)$ have modulus one and are simple.

Remark 1. The idea to use different discretizations for different parts of the differential equation is not new. Already Dahlquist [5, Chapter 7] considers stable combinations of two multistep schemes for the solution of second order differential equations. Often, the vector field is split into a sum of two vector fields (stiff and nonstiff), cf. [2]. In the context of differential-algebraic equations, the differential and algebraic parts can be treated by different methods, cf. [3]. An essential difference of these approaches to the present work is the use of symmetric methods with the aim of preserving a qualitatively correct long-time behavior of the numerical approximation.

1.2 Known results about the long-time behavior

Classical convergence estimates are usually of the form (3), where $C(T) = e^{LT}$ and L is proportional to a Lipschitz constant of the differential equation. They give information only on intervals of length $\mathcal{O}(1)$. Different techniques, usually based on a kind of backward error analysis, are required to get insight into the long-time behavior (e.g., energy-preservation or error growth for nearly integrable systems) of the numerical solution.

From one-step methods it is known that symplecticity and/or symmetry of the numerical integrator play an important role in the long-time behavior of numerical approximations for Hamiltonian systems. This motivates the consideration of symmetric multistep methods. However, already Dahlquist [5, p. 52] pointed out the danger of applying symmetric multistep methods for long-time integration, when he writes[1] "then the unavoidable weak instability arising from the root $\zeta = -1$ of $\rho(\zeta)$ may make [such methods] inferior to methods with a lower value of p in integrations over a long range". Also the analysis of [7] indicates that symmetric multistep methods (applied to the whole differential system) are usually not reliable for integrations over long times. This is the reason why we are mainly interested in partitioned multistep methods, where the characteristic polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ do not have common zeros with the exception of $\zeta = 1$.

For separable Hamiltonian systems with

$$H(p,q) = \frac{1}{2}\, p^{\mathsf{T}} M^{-1} p + U(q), \tag{5}$$

where M is a constant, symmetric, positive definite matrix, the long-time behavior of linear multistep methods is well understood. In this case the differential equation reduces to the second order problem $\ddot{q} = -M^{-1}\nabla U(q)$. Also in the partitioned multistep method the presence of the momenta p_n can be eliminated, which yields

$$\sum_{j=0}^{2k} \alpha_j^{(2)} q_{n+j} = -h^2 \sum_{j=0}^{2k} \beta_j^{(2)} M^{-1} \nabla U(q_{n+j}), \tag{6}$$

where the generating polynomial $\rho_2(\zeta), \sigma_2(\zeta)$ of the coefficients $\alpha_j^{(2)}, \beta_j^{(2)}$ are related to those of (2) by

$$\rho_2(\zeta) = \rho_p(\zeta)\rho_q(\zeta), \qquad \sigma_2(\zeta) = \sigma_p(\zeta)\sigma_q(\zeta).$$

Formula (6) permits the computation of $\{q_n\}$ independent of velocity and momenta. They can be computed a posteriori by a finite difference formula of the form

$$p_n = \frac{1}{h} \sum_{j=-l}^{l} \delta_j M\, q_{n+j}. \tag{7}$$

[1] We thank Gustaf Söderlind for drawing our attention to this part of Dahlquist's thesis.

This is a purely local approach, which does not influence the propagation of the numerical solution, and therefore has no effect on its long-time behavior.

We now present a few interesting results from the publication [9] about the long-time behavior of numerical solutions. This article considers linear multistep methods (6), which do not necessarily originate from a partitioned method (2), together with local approximations of the momenta. Assumptions on the method (6) are the following:

(A1) it is of order r, i.e., $\rho_2(\zeta)/(\log\zeta)^2 - \sigma_2(\zeta) = \mathscr{O}((\zeta-1)^r)$ for $\zeta \to 1$,
(A2) it is symmetric, i.e., $\rho_2(\zeta) = \zeta^k \rho_2(1/\zeta)$ and $\sigma_2(\zeta) = \zeta^k \sigma_2(1/\zeta)$,
(A3) it is s-stable, i.e., apart from the double zero at 1, all zeros of $\rho_2(\zeta)$ are simple and of modulus one.

Under these assumptions we have the following results on the long-time behavior:

- the total energy (5) is preserved up to $\mathscr{O}(h^r)$ over times $\mathscr{O}(h^{-r-2})$, i.e.,

$$H(p_n,q_n) = H(p_0,q_0) + \mathscr{O}(h^r) \quad \text{for} \quad nh \le h^{-r-2},$$

- quadratic first integrals of the form $L(p,q) = p^{\mathsf{T}} A\, q$ are nearly preserved:

$$L(p_n,q_n) = L(p_0,q_0) + \mathscr{O}(h^r) \quad \text{for} \quad nh \le h^{-r-2},$$

- for integrable reversible systems (under suitable assumptions, see [9]) we have for the angle variable $\Theta(p,q)$ and the action variable $I(p,q)$ the estimates

$$\begin{aligned} \Theta(p_n,q_n) &= \Theta(p_0,q_0) + \mathscr{O}(t\,h^r) \\ I(p_n,q_n) &= I(p_0,q_0) + \mathscr{O}(h^r) \end{aligned} \quad \text{for} \quad 0 \le t = nh \le h^{-r}.$$

The constants symbolized by $\mathscr{O}$ are independent of n and h.

1.3 Numerical experiments

For systems with Hamiltonian (5), partitioned linear multistep methods of the form (2) have the same long-time behavior as linear multistep methods for second order problems (Section 1.2) even if the derivative approximation is not given locally by a finite difference formula as in (7). The aim of this section is to get some insight into the long-time behavior of partitioned linear multistep methods (2) applied to Hamiltonian systems that are more general than (5).

Separable Hamiltonian systems. Let us first consider separable polynomial Hamiltonians $H(p,q) = T(p) + U(q)$, where

$$T(p) = \sum_{2\le j+k\le 3} a_{jk}\, p_1^j\, p_2^k + \big(p_1^4 + p_2^4\big), \quad U(q) = \sum_{2\le j+k\le 3} b_{jk}\, q_1^j\, q_2^k + \big(q_1^4 + q_2^4\big).$$

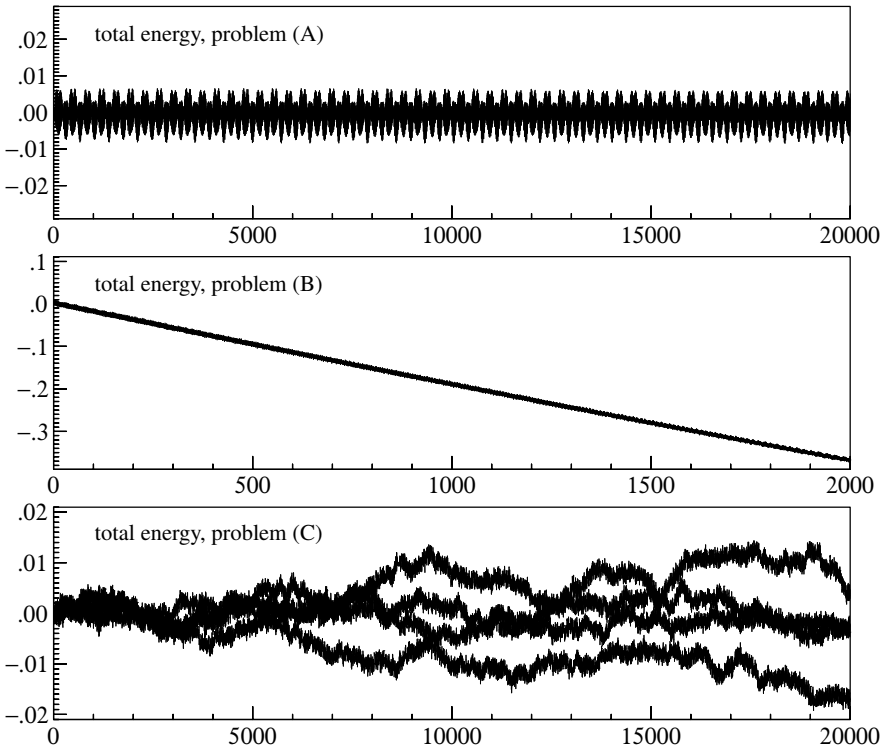


Fig. 1 Numerical Hamiltonian of method 'plmm2' applied with step size $h = 0.005$ for problems (A) and (B), and with $h = 001$ for problem (C); initial values $q_1(0) = 1$, $q_2(0) = -1.2$, $p_1(0) = 0.2$, $p_2(0) = -0.9$. Starting approximations are computed with high precision.

The positive definite quartic terms imply that solutions remain in a compact set. We consider the following three situations:

(A) Non-vanishing coefficients are $a_{02} = 1$, $a_{20} = 1$, and $b_{02} = 2$, $b_{20} = 1$, $b_{03} = 1$. Since $T(-p) = T(p)$, the system is reversible with respect to $p \leftrightarrow -p$. Moreover, it is separated into two systems with one degree of freedom.

(B) Non-vanishing coefficients are $a_{02} = 1$, $a_{20} = 1$, $a_{03} = 1$, $a_{30} = -0.5$, and $b_{02} = 2$, $b_{20} = 1$, $b_{03} = 1$. The system is not reversible, but still equivalent to two systems with one degree of freedom.

(C) Non-vanishing coefficients are $a_{02} = 1$, $a_{20} = 1$, and $b_{02} = 2$, $b_{20} = 1$, $b_{12} = -1$, $b_{21} = 2$. The system is reversible, and it is a coupled system with two degrees of freedom.

We consider the following partitioned linear multistep methods:

Table 1 Numerical energy behavior on intervals of length $\mathcal{O}(h^{-2})$; t is time, h the step size.

method	problem (A)	problem (B)	problem (C)
plmm2, order 2	$\mathcal{O}(h^2)$	$\mathcal{O}(th^2)$	$\mathcal{O}(\sqrt{t}\,h^2)$
plmm4, order 4	$\mathcal{O}(h^4)$	$\mathcal{O}(th^4)$	$\mathcal{O}(h^4)$
plmm4c, order 4	$\mathcal{O}(h^4)$	$\mathcal{O}(h^4+th^6)$	$\mathcal{O}(h^4)$

plmm2
$$\rho_p(\zeta)=(\zeta-1)(\zeta+1) \qquad \sigma_p(\zeta)=2\zeta$$
$$\rho_q(\zeta)=(\zeta-1)(\zeta^2+1) \qquad \sigma_q(\zeta)=\zeta^2+\zeta$$

plmm4
$$\rho_p(\zeta)=\zeta^4-1 \qquad \sigma_p(\zeta)=\frac{4}{3}\big(2\zeta^3-\zeta^2+2\zeta\big)$$
$$\rho_q(\zeta)=\zeta^5-1 \qquad \sigma_q(\zeta)=\frac{5}{24}\big(11\zeta^4+\zeta^3+\zeta^2+11\zeta\big)$$

Figure 1 shows the numerical Hamiltonian for the second order method 'plmm2', and Table 1 presents the qualitative behavior in dependence of time and step size. Looking at Figure 1, we notice that this partitioned multistep method behaves very similar to (non-symplectic) symmetric one-step methods, as can be seen from the experiments of [11]. For non-reversible problems without any symmetry we have a linear growth in the energy, for reversible problems we observe boundedness for integrable systems and for problems with one degree of freedom, and we observe a random walk behavior of the numerical energy for chaotic solutions. This is illustrated by plotting the numerical Hamiltonian of 4 trajectories with randomly perturbed initial values (perturbation of size $\approx 10^{-15}$) for problem (C).

The intervals considered in the experiments of Figure 1 are relatively short. What happens on longer time intervals? For problem (A), the numerical energy of the method 'plmm2' shows the same regular, bounded, $\mathcal{O}(h^2)$ behavior on intervals as long as 10^7. No secular terms and no influence of parasitic components can be observed. For problem (B) the linear error growth in the energy as $\mathcal{O}(th^2)$ can be observed on intervals of length $\mathcal{O}(h^{-2})$. The behavior for problem (C) is shown in Figure 2. We observe that after a time that is proportional to h^{-2} (halving the step size increases the length of the interval by a factor four) an exponential error growth is superposed to the random walk behavior of Figure 1. Such a behavior is

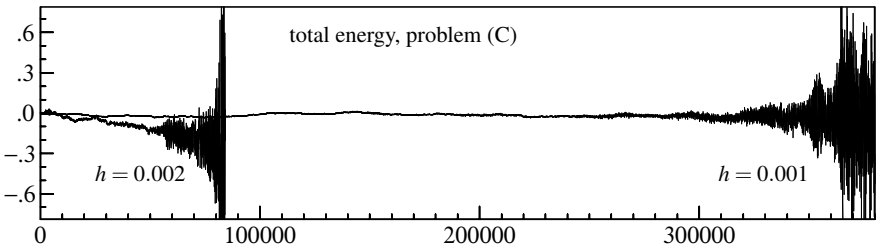


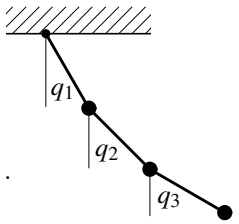
Fig. 2 Numerical Hamiltonian of method 'plmm2' for problem (C); data as in Figure 1, but on a longer time interval.

not possible for symmetric one-step methods. It will be explained by the presence of parasitic solution components.

We have repeated all experiments with the fourth order partitioned linear multistep method 'plmm4' with characteristic polynomials given at the beginning of this section. Table 1 shows the behavior on intervals of length $\mathscr{O}(h^{-2})$. Whereas the behavior for problems (A) and (B) is expected, we cannot observe a random walk behavior for problem (C). On very long time intervals, the energy error remains nicely bounded of size $\mathscr{O}(h^4)$ for the problem (A). For the problems (B) and (C), however, an exponential error growth like $\delta\exp(ch^2t)$ with small δ is superposed, which becomes visible after an interval of length $\mathscr{O}(h^{-2})$. Consequently, the exponent two in the length of the interval is not related to the order of the method.

Triple pendulum. For non-separable Hamiltonians, symmetric and/or symplectic one-step methods are in general implicit. It is therefore of interest to study the behavior of explicit symmetric multistep methods applied to such systems. We consider the motion of a triple pendulum, which leads to a Hamiltonian system with

$$H(p,q) = \frac{1}{2}\,p^{\mathsf{T}}M(q)^{-1}p + U(q),$$



where $U(q) = -3\cos q_1 - 2\cos q_2 - \cos q_3$ and

$$M(q) = \begin{pmatrix} 3 & 2\cos(q_2-q_1) & \cos(q_3-q_1) \\ 2\cos(q_2-q_1) & 2 & \cos(q_3-q_2) \\ \cos(q_3-q_1) & \cos(q_3-q_2) & 1 \end{pmatrix}.$$

This matrix is positive definite with $\det M(q) = 4 - 2\cos^2(q_2-q_1) - \cos^2(q_3-q_2)$. We have experimented with both partitioned multistep methods (order 2 and order 4) and we observed that the methods give excellent results when the angles are not to large, and the motion is not too chaotic.

For example, if we take initial values $q_1(0) = \pi/12$, $q_2(0) = \pi/6$, for $q_3(0)$ a value between 0 and $5\pi/12$, and zero initial values for the velocities, then the error in the Hamiltonian is of size $\mathscr{O}(h^2)$ (for 'plmm2') and $\mathscr{O}(h^4)$ (for 'plmm4') without any drift. This has been verified numerically on an interval $[0, 10^7]$. Changing the initial value for $q_3(0)$ to $-\pi/12$ shows an exponential increase of the error after $t \approx 4\cdot 10^6$, and a change to $6\pi/12$ shows such a behavior already at $t \approx 4000$.

Ablowitz–Ladik discrete nonlinear Schrödinger equation. As an example of a completely integrable lattice equation we consider the Ablowitz–Ladik discrete nonlinear Schrödinger equation (see [1])

$$\mathrm{i}\,\dot{u}_k + \frac{1}{\Delta x^2}\big(u_{k+1} - 2u_k + u_{k-1}\big) + |u_k|^2(u_{k+1} + u_{k-1}) = 0,$$

under periodic boundary conditions $u_{k+N} = u_k$, where $\Delta x = L/N$. Separating real and imaginary parts in the solution $u_k = p_k + \mathrm{i}\,q_k$, the equation becomes

$$\begin{aligned} \dot{p}_k &= -\frac{1}{\Delta x^2}\big(q_{k+1} - 2q_k + q_{k-1}\big) - (p_k^2 + q_k^2)(q_{k+1} + q_{k-1}) \\ \dot{q}_k &= \frac{1}{\Delta x^2}\big(p_{k+1} - 2p_k + p_{k-1}\big) + (p_k^2 + q_k^2)(p_{k+1} + p_{k-1}) \end{aligned} \tag{8}$$

with boundary conditions $p_{k+N} = p_k$ and $q_{k+N} = q_k$. This system can be written in the non-canonical Hamiltonian form

$$\dot{p} = -D(p,q)\,\nabla_q H(p,q), \qquad \dot{q} = D(p,q)\,\nabla_p H(p,q),$$

where $D(p,q)$ is the diagonal matrix with entries $d_k(p,q) = \frac{1}{\Delta x}(1 + \Delta x^2(p_k^2 + q_k^2))$, and the Hamiltonian is given by

$$H(p,q) = \frac{1}{\Delta x}\sum_{k=1}^{N}\big(p_k p_{k-1} + q_k q_{k-1}\big) - \frac{1}{\Delta x^3}\sum_{k=1}^{N}\ln\big(1 + \Delta x^2(p_k^2 + q_k^2)\big). \tag{9}$$

Furthermore, the expression

$$I(p,q) = \frac{1}{\Delta x}\sum_{k=1}^{N}\big(p_k p_{k-1} + q_k q_{k-1}\big) \tag{10}$$

is a first integral of the system (8). Since the system is completely integrable, there are in addition $N-2$ other independent first integrals.

Since we are confronted with a Poisson system with non-separable Hamiltonian, there do not exist symplectic and/or symmetric integrators that are explicit. It is therefore of high interest to study the performance of explicit partitioned linear multistep methods, when applied to the system (8). Notice that the system is reversible with respect to the symmetries $p \leftrightarrow -p$ and $q \leftrightarrow -q$. Following [16, 13], we consider initial values

$$p_k(0) = \frac{1}{2}\big(1 - \varepsilon\cos(bx_k)\big), \qquad q_k(0) = 0, \tag{11}$$

where $x_k = -L/2 + (k-1)\Delta x$, $\Delta x = L/N$, $b = 2\pi/L$ with $L = 2\pi\sqrt{2}$, and $\varepsilon = 0.01$. We apply the second order method 'plmm2' to the system with $N = 16$, and we use various time step sizes for integrations over long time intervals. Figure 3 shows the error in both first integrals, H and I, to the left on the first subinterval of length 50, and to the right on the final subinterval starting at $t = 10^6$. We observe that halving the step size decreases the error by a factor of $4 = 2^2$, which is in accordance with a second order integrator. Similar to an integration with a symplectic scheme, the partitioned multistep method behaves very well over long times and no drift in the invariants can be seen. Comparing the results for different step sizes at the final interval, we notice a time shift in the numerical solution, but amplitude and shape of the oscillations are not affected. We also observe that the errors are a superposition of a slowly varying function scaled with h^2, and of high oscillations that decrease faster than with a factor 4, when the step size is halved.

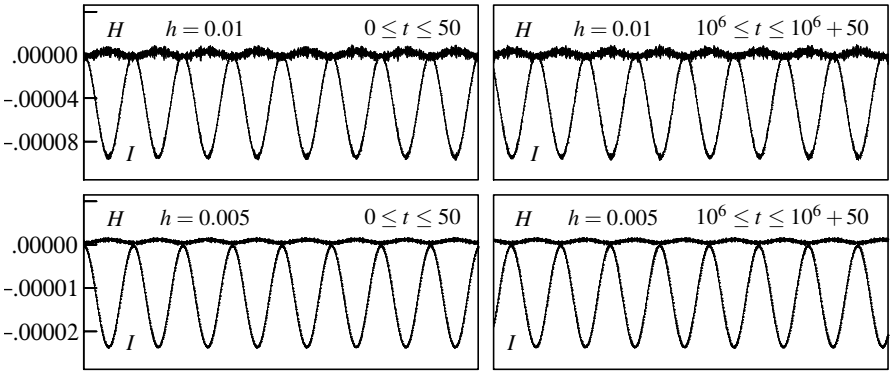


Fig. 3 Numerical preservation of the invariants H and I, defined in (9) and (10), with the method 'plmm2' applied with step sizes $h = 0.01$ and $h = 0.005$; initial data are that of (11).

The same qualitative behavior can be observed with the 4th order, explicit, partitioned multistep method 'plmm4' for step sizes smaller than $h = 0.005$. As expected, the error decreases by a factor of $16 = 2^4$ when having the step size. For larger values of ε, say $\varepsilon \geq 0.05$ the behavior of the partitioned multistep method is less regular.

Further numerical experiments can be found in [7]. Excellent long-time behavior of partitioned linear multistep methods is reported for the Kepler problem and for a test problem in molecular dynamics simulation (frozen Argon crystal). Exponentially fitted partitioned linear multistep methods are considered in [18] for the long-term integration of N-body problems.

2 Long-time analysis of the underlying one-step method

For one-step methods, the long-time behavior of numerical approximations is easier to analyze than for multistep methods. Whereas the notions of symplecticity and energy preservation are straightforward for one-step methods, this is not the case for multistep methods. It has been shown by Kirchgraber [14] that the numerical solution of strictly stable[2] linear multistep methods essentially behaves like that of a one-step method, which we call *underlying one-step method*. For a fixed step size h and a differential equation $\dot{y} = f(y)$, it is defined as the mapping $\Phi_h(y)$, such that the sequence defined by $y_{n+1} = \Phi_h(y_n)$ satisfies the multistep formula. This means that for starting approximations given by $y_j = \Phi_h^j(y_0)$ for $j = 0, 1, \ldots, k-1$, the numerical approximations obtained by the multistep formula coincides with that of the underlying one-step method (neglecting round-off effects).

[2] A linear multistep is called strictly stable, if $\zeta_1 = 1$ is a simple zero of the ρ polynomial, and all other zeros have modulus strictly smaller than one.

For symmetric linear multistep methods, which cannot be strictly stable, such an underlying one-step method exists as a formal series in powers of h (see [6, page 274] and [10, Sect. XV.2.2]). Despite its non-convergence, it can give much insight into the long-time behavior of the method.

2.1 Analysis for the harmonic oscillator

Consider a harmonic oscillator, written as a first order Hamiltonian system,

$$\begin{aligned} \dot p &= -\omega\, q, \qquad & p(0) &= p_0, \\ \dot q &= \omega\, p, \qquad & q(0) &= q_0. \end{aligned}$$

Applying the partitioned linear multistep method (2) to this system yields the difference equations

$$\rho_p(E)\, p_n = -\omega h\, \sigma_p(E)\, q_n, \qquad \rho_q(E)\, q_n = \omega h\, \sigma_q(E)\, p_n, \tag{12}$$

where we have made use of the shift operator $Ey_n = y_{n+1}$. Looking for solutions of the form $p_n = a\zeta^n$, $q_n = b\zeta^n$ we are led to the 2-dimensional linear system

$$R(\omega h, \zeta) \begin{pmatrix} a \\ b \end{pmatrix} = 0 \qquad \text{with} \qquad R(\omega h, \zeta) = \begin{pmatrix} \rho_p(\zeta) & \omega h\, \sigma_p(\zeta) \\ -\omega h\, \sigma_q(\zeta) & \rho_q(\zeta) \end{pmatrix}. \tag{13}$$

It has a nontrivial solution if and only if $\det R(\omega h, \zeta) = 0$. For small values of ωh the roots of this equation are close to the zeros of the polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$. By consistency we have two roots close to 1, they are conjugate to each other, and they satisfy $\zeta_0 = \zeta_0(\omega h) = 1 + \mathrm{i}\omega h + \mathscr{O}(h^2)$ and $\overline{\zeta}_0 = \overline{\zeta}_0(\omega h) = 1 - \mathrm{i}\omega h + \mathscr{O}(h^2)$ (principal roots). They lead to approximations to the exact solution, which is a linear combination of $\mathrm{e}^{\mathrm{i}\omega t}$ and $\mathrm{e}^{-\mathrm{i}\omega t}$. The other roots lead to parasitic terms in the numerical approximations. The general solution $(p_n, q_n)^{\mathsf{T}}$ of the difference equation (12) is in fact a linear combination of $\zeta^n (a,b)^{\mathsf{T}}$, where ζ is a root of $\det R(\omega h, \zeta) = 0$, and the vector $(a,b)^{\mathsf{T}}$ satisfies the linear system (13).

Underlying one-step method. We consider a numerical solution of (12) that is built only on linear combinations of ζ_0^n and $\overline{\zeta}_0^n$. It has to be of the form

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = \Phi_n \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}, \qquad \Phi_n = \tfrac{1}{2}\big(\zeta_0^n + \overline{\zeta}_0^n\big)\, I + \tfrac{1}{2\mathrm{i}}\big(\zeta_0^n - \overline{\zeta}_0^n\big)\, C, \tag{14}$$

where the matrix C satisfies $R_0(I - \mathrm{i}C) = 0$ and $\overline{R}_0(I + \mathrm{i}C) = 0$, so that the vectors multiplying ζ_0^n and $\overline{\zeta}_0^n$ satisfy the relation (13) with $R_0 = R(\omega h, \zeta_0)$. It follows from the consistency of the method that for small but nonzero ωh the real and imaginary parts of the matrix R_0 are invertible. This permits us to compute the real matrix $C = -\mathrm{i}\,(R_0 + \overline{R}_0)^{-1}(R_0 - \overline{R}_0)$. As a consequence of $R_0 = \frac{1}{2}(R_0 + \overline{R}_0)(I + \mathrm{i}C)$ and

$\det R_0 = 0$ we have $\det C = 1$ and $\operatorname{trace} C = 0$, which implies $C^2 = -I$. The matrix Φ_n of (14) thus satisfies $\Phi_{n+1} = \Phi_n \Phi_1$, and consequently $\Phi_n = \Phi_1^n$, so that the underlying one-step method is seen to be given by

$$\begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix} = \Phi(\omega h) \begin{pmatrix} p_n \\ q_n \end{pmatrix}, \qquad \Phi(\omega h) = \frac{1}{2}\big(\zeta_0 + \overline{\zeta}_0\big) I + \frac{1}{2\mathrm{i}}\big(\zeta_0 - \overline{\zeta}_0\big) C. \tag{15}$$

Notice that $\Phi(\omega h)$ is not an analytic function of ωh.

Properties of the underlying one-step method. The above derivation is valid for all partitioned multistep methods. If the method is symmetric, also the coefficients of the polynomial $\det R(h\omega, \zeta)$ are symmetric, so that with $\zeta_0 = \zeta_0(\omega h)$ also its inverse is a solution of $\det R(h\omega, \zeta) = 0$. This implies $\zeta_0^{-1} = \overline{\zeta}_0$, and hence also $|\zeta_0| = 1$. Similarly, the symmetry of the methods (ρ_p, σ_p) and (ρ_q, σ_q) imply that $C(-\omega h) = C(\omega h)$. Consequently, we have $\Phi(-\omega h)\Phi(\omega h) = I$, which proves the *symmetry* of the underlying one-step method.

Furthermore, the mapping defined by the matrix $\Phi(\omega h)$ is *symplectic*:

$$\Phi(\omega h)^{\mathsf{T}} J \, \Phi(\omega h) = J \qquad \text{with} \qquad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{16}$$

This follows from the relations $C^{\mathsf{T}} J + J C = 0$ and $C^T J C = J$, which are a consequence of $\det C = 1$ and $\operatorname{trace} C = 0$.

Since the eigenvalues of C are $\pm\mathrm{i}$, we have

$$T C T^{-1} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \text{with} \qquad T = \begin{pmatrix} 1 & 0 \\ a & b \end{pmatrix},$$

where (a, b) is the first row of the matrix C. Notice that we have $a = \mathscr{O}((\omega h)^2)$ and $b = 1 + \mathscr{O}((\omega h)^2)$. This transformation implies that $T\Phi(\omega h)T^{-1}$ is an orthogonal matrix, so that

$$\frac{\omega}{2} \left\| T \begin{pmatrix} p_n \\ q_n \end{pmatrix} \right\|^2 = \frac{\omega}{2} \left(p_n^2 + (a p_n + b q_n)^2 \right)$$

is a conserved quantity that is $\mathscr{O}(h^2)$ close to the true Hamiltonian.

Parasitic solution components. The complete solution of the difference equation (12) is given by

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = \Phi_1(\omega h)^n \begin{pmatrix} a \\ b \end{pmatrix} + \sum_{l=1}^{2k-2} \zeta_l(\omega h)^n \begin{pmatrix} a_l \\ b_l \end{pmatrix},$$

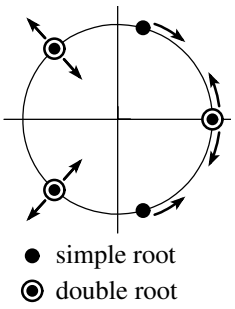
where $\zeta_l(\omega h)$ are the roots of $\det R(\omega h, \zeta) = 0$ which are different from the principal roots $\zeta_0(\omega h)$ and $\overline{\zeta}_0(\omega h)$. They are called parasitic roots of the method. Initial approximations (p_j, q_j) for $j = 0, 1, \ldots, k-1$ uniquely determine the vectors (a, b) and (a_l, b_l), recalling that (a_l, b_l) has to satisfy the relation (13).

If the starting values (p_j, q_j) approximate for $j = 0, 1, \ldots, k-1$ the exact solution $(p(t_0 + jh), q(t_0 + jh))$ up to an error of size $\mathscr{O}(h^{\nu+1})$ with $\nu \le r$, then we have

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} + \mathscr{O}(h^{\nu+1}), \qquad \begin{pmatrix} a_l \\ b_l \end{pmatrix} = \mathscr{O}(h^{\nu+1}) \qquad \text{for all } l.$$

For zero-stable multistep methods, all roots of $\det R(\omega h, \zeta) = 0$ can be bounded by $|\zeta_l(\omega h)| \le 1 + \gamma\omega h$ (here $\gamma > 0$ and $\omega > 0$). This implies that $|\zeta_l(\omega h)^n| \le \mathrm{e}^{\gamma\omega T}$ for $nh \le T$, and the parasitic solution components remain small of size $\mathscr{O}(h^{\nu+1})$ on intervals of fixed length. To have a similar estimate on arbitrarily long intervals, the roots $\zeta_l(\omega h)$ have to be bounded by 1.

In general, we do not have a control on the modulus of ζ_l. However, for symmetric methods we know that with ζ_l not only the complex conjugate $\overline{\zeta}_l$, but also the inverse ζ_l^{-1} are roots of $\det R(\omega h, \zeta) = 0$. Furthermore, the roots $\zeta_l(\omega h)$ depend continuously on its argument. If $\zeta_l(0)$ is a double root of $\det R(0, \zeta) = 0$, then it is possible that it splits for $\omega h > 0$ into a pair of roots, one of which has modulus larger than 1, and one smaller than 1 (see the figure). If $\zeta_l(0)$ is a simple root, then we must have $\overline{\zeta}_l(\omega h) = \zeta_l(\omega h)^{-1}$, implying $|\zeta_l(\omega h)| = 1$ for sufficiently small $\omega h > 0$.



Consequently, if apart from the double root at 1, all roots of $\det R(0, \zeta) = 0$ are simple (i.e., with the exception of 1, all zeros of $\rho_p(\zeta)$ are different from those of $\rho_q(\zeta)$), the parasitic solution components remain bounded of size $\mathscr{O}(h^{\nu+1})$ independent of the length of the integration interval.

Linear change of coordinates. Partitioned linear multistep methods are invariant with respect to linear transformations of the form $\tilde{p} = T_p\, p$, $\tilde{q} = T_q\, q$. However, care has to be taken when p and q components are mixed. Suppose, for example, that after such a transformation the harmonic oscillator reduces to a Hamiltonian system with (we put $\omega = 1$ for convenience)

$$H(p,q) = \tfrac{1}{2}\big(p^2 + 2\,\varepsilon\, p\, q + q^2\big),$$

where $\varepsilon \neq 0$ is a small parameter. An application of the partitioned multistep method yields the difference equation

$$\begin{aligned} \rho_p(E)\, p_n &= -h\,\big(\varepsilon\, \sigma_p(E)\, p_n + \sigma_p(E)\, q_n\big), \\ \rho_q(E)\, q_n &= h\,\big(\sigma_q(E)\, p_n + \varepsilon\, \sigma_q(E)\, q_n\big). \end{aligned} \tag{17}$$

Instead to (13) we are led this time to the system

$$R(h,\zeta)\begin{pmatrix} a \\ b \end{pmatrix} = 0 \quad \text{with} \quad R(h,\zeta) = \begin{pmatrix} \rho_p(\zeta) + \varepsilon h \sigma_p(\zeta) & h\,\sigma_p(\zeta) \\ -h\,\sigma_q(\zeta) & \rho_q(\zeta) - \varepsilon h \sigma_q(\zeta) \end{pmatrix}.$$

Even if we only consider symmetric partitioned linear multistep methods, the coefficients of the polynomial $\det R(h,\zeta)$ are no longer symmetric, so that the modulus of its zeros is in general not equal to one. A straightforward computation shows that

for simple roots of $R(0,\zeta)=0$ (for example if we have $\rho_p(\zeta_l)=0$ but $\rho_q(\zeta_l)\neq 0$), the continuous continuation satisfies

$$\zeta_l(h)=\zeta_l\big(1-\mu_l\varepsilon h+\mathscr{O}(h^2)\big),\qquad \mu_l=\frac{\sigma_p(\zeta_l)}{\zeta_l\,\rho_p(\zeta_l)}.$$

From the symmetry of the method it follows that μ_l is a real number. It is called growth parameter. We conclude from this asymptotic formula that $|\zeta_l(h)|>1$ for small h, if the product $\mu_l\varepsilon$ is negative. In such a situation parasitic solution components grow exponentially with time, and the numerical solution becomes meaningless on integration intervals whose length T is such that $h^{\nu+1}\mathrm{e}^{-\mu_l\varepsilon T}\geq 1$.

2.2 Backward error analysis (smooth numerical solution)

An important tool for the study of the long-time behavior of numerical approximations is 'backward error analysis'. The idea is to interpret the numerical solution of a one-step method as the exact solution of a modified differential equation (for details see Chapter IX of [10]). For linear multistep methods, it is in principle possible to construct the underlying one-step method as a formal series in powers of the step size h, and then to apply the well-established techniques. Here, we follow the approach of [7, 9], where the modified differential equation is directly obtained from the multistep schemes without passing explicitly through the underlying one-step method.

Theorem 1 (modified differential equation). *Consider a consistent, partitioned linear multistep method (2), applied to a partitioned system (1). There then exist h-independent functions $f_j(p,q)$, $g_j(p,q)$, such that for every truncation index N every solution $p_h(t),q_h(t)$ of the system*

$$\begin{aligned}\dot p &= f(p,q)+hf_1(p,q)+\ldots+h^{N-1}f_{N-1}(p,q)\\ \dot q &= g(p,q)+hg_1(p,q)+\ldots+h^{N-1}g_{N-1}(p,q)\end{aligned}\tag{18}$$

satisfies the multistep formula up to a defect of size $\mathscr{O}(h^{N+1})$, i.e.,

$$\begin{aligned}\sum_{j=0}^{k}\alpha_j^p\,p_h(t+jh) &= h\sum_{j=0}^{k}\beta_j^p\,f\big(p_h(t+jh),q_h(t+jh)\big)+\mathscr{O}(h^{N+1})\\ \sum_{j=0}^{k}\alpha_j^q\,q_h(t+jh) &= h\sum_{j=0}^{k}\beta_j^q\,g\big(p_h(t+jh),q_h(t+jh)\big)+\mathscr{O}(h^{N+1}).\end{aligned}\tag{19}$$

The constant symbolized by $\mathscr{O}$ is independent of h, but depends on the truncation index N. It also depends smoothly on t. If the method is of order r, then we have $f_j(p,q)=g_j(p,q)=0$ for $1\leq j<r$.

Proof. We closely follow the proof for second order equations in [9]. Denoting time differentiation by D, the Taylor series expansion of a function can be written as $y(t+h) = \mathrm{e}^{hD} y(t)$. The equations (19) thus become

$$\begin{aligned} \rho_p(\mathrm{e}^{hD}) p_h(t) &= h\,\sigma_p(\mathrm{e}^{hD}) f\big(p_h(t), q_h(t)\big) + \mathscr{O}(h^{N+1}) \\ \rho_q(\mathrm{e}^{hD}) q_h(t) &= h\,\sigma_q(\mathrm{e}^{hD}) g\big(p_h(t), q_h(t)\big) + \mathscr{O}(h^{N+1}). \end{aligned} \tag{20}$$

With the coefficients of the expansions

$$\frac{x\,\sigma_p(\mathrm{e}^x)}{\rho_p(\mathrm{e}^x)} = 1 + \mu_1^p x + \mu_2^p x^2 + \ldots, \qquad \frac{x\,\sigma_q(\mathrm{e}^x)}{\rho_q(\mathrm{e}^x)} = 1 + \mu_1^q x + \mu_2^q x^2 + \ldots, \tag{21}$$

this becomes equivalent to (omitting the argument t)

$$\begin{aligned} \dot{p}_h &= \big(1 + \mu_1^p hD + \mu_2^p h^2 D^2 + \ldots\big) f(p_h, q_h) + \mathscr{O}(h^N) \\ \dot{q}_h &= \big(1 + \mu_1^q hD + \mu_2^q h^2 D^2 + \ldots\big) g(p_h, q_h) + \mathscr{O}(h^N). \end{aligned} \tag{22}$$

For a function $\Psi(p,q)$, we have

$$D\Psi(p_h, q_h) = \partial_p \Psi(p_h, q_h) f_h(p_h, q_h) + \partial_q \Psi(p_h, q_h) g_h(p_h, q_h),$$

where the functions $f_h(p,q)$ and $g_h(p,q)$ are an abbreviation for the right-hand side of (18). Applying this formula iteratively to the expressions in (22) and collecting equal powers of h, a comparison of the equations (18) and (22) determines recursively the functions $f_j(p,q)$ and $g_j(p,q)$. □

The flow of the modified differential equation (18) depends on the parameter h. If we denote this flow by $\varphi_t^{[h]}(p,q)$, then the underlying one-step method of the partitioned linear multistep method is given by $\Phi_h(p,q) = \varphi_h^{[h]}(p,q)$ up to an error of size $\mathscr{O}(h^{N+1})$.

Corollary 1. *Assume that the partitioned linear multistep method is symmetric, i.e., both multistep schemes satisfy the symmetry relations (4). We then have:*

a) The expansion of the vector field of the modified differential equation (18) is in even powers of h.

b) If the differential equation (1) is reversible, i.e., $f(-p,q) = f(p,q)$ and $g(-p,q) = -g(p,q)$, then the modified differential equation (18) is also reversible.

Proof. The symmetry relations (4) imply that the expressions of (21) are even functions of x. This proves statement (a).

If $\big(f_h(p,q), g_h(p,q)\big)$ is a reversible vector field, then the function $D^2\Psi(p,q)$ has the same parity in p as the function $\Psi(p,q)$. As a consequence of the recursive construction of the modified differential equation, and of the fact that only even powers of D appear in (22), this observation proves the statement (b). □

Theorem 1 tells us that the solution of the truncated modified differential equation (18) satisfies the multistep formulas up to a defect of size $\mathscr{O}(h^{N+1})$. Consequently,

the classical analysis shows that on intervals of length $T = \mathscr{O}(1)$,

$$\|p_n - p_h(nh)\| + \|q_n - q_h(nh)\| \leq C(T)\, h^N.$$

2.3 Near energy preservation

Whereas the analysis of the previous Section 2.2 is valid for general partitioned differential equations, we assume here that the vector field is Hamiltonian and given by

$$f(p,q) = -\nabla_q H(p,q), \qquad g(p,q) = \nabla_p H(p,q). \tag{23}$$

In this situation the exact solution satisfies $H\big(p(t),q(t)\big) = \text{const}$, and it is of interest to study whether numerical approximations of partitioned linear multistep methods (nearly) preserve the energy $H(p,q)$ over long times. Recall that in this chapter we consider only 'smooth' numerical solutions, which are given by the flow of the modified differential equation (18) up to an arbitrarily small error of size $\mathscr{O}(h^N)$. We therefore have to investigate the near preservation of $H\big(p_h(t),q_h(t)\big)$.

The solution of the truncated modified equation satisfies (20). Instead of dividing by the ρ polynomial, which led us to the construction of the modified differential equation, we divide the relation by the σ polynomial. This leads to

$$\begin{aligned} \big(1 + \lambda_1^p hD + \lambda_2^p h^2 D^2 + \ldots\big)\dot{p}_h &= -\nabla_q H(p_h,q_h) + \mathscr{O}(h^N) \\ \big(1 + \lambda_1^q hD + \lambda_2^q h^2 D^2 + \ldots\big)\dot{q}_h &= \nabla_p H(p_h,q_h) + \mathscr{O}(h^N), \end{aligned} \tag{24}$$

where the coefficients in the expansion are given by

$$\frac{\rho_p(\mathrm{e}^x)}{x\,\sigma_p(\mathrm{e}^x)} = 1 + \lambda_1^p x + \lambda_2^p x^2 + \ldots, \qquad \frac{\rho_q(\mathrm{e}^x)}{x\,\sigma_q(\mathrm{e}^x)} = 1 + \lambda_1^q x + \lambda_2^q x^2 + \ldots\,. \tag{25}$$

For symmetric methods, we are concerned with even functions of x, so that the expansions in (24) are in even powers of h. In this situation we multiply the first relation of (24) with $\dot{q}_h$, the second one with $\dot{p}_h$, and we subtract both so that the right-hand side becomes a total differential. This yields

$$\dot{q}_h^{\mathsf{T}}\big(1 + \lambda_2^p h^2 D^2 + \ldots\big)\dot{p}_h - \dot{p}_h^{\mathsf{T}}\big(1 + \lambda_2^q h^2 D^2 + \ldots\big)\dot{q}_h + \frac{\mathrm{d}}{\mathrm{d}t} H\big(p_h,q_h\big) = \mathscr{O}(h^N). \tag{26}$$

The main ingredient for a further simplification is the fact that

$$\dot{q}_h^{\mathsf{T}} p_h^{(2j+1)} - \dot{p}_h^{\mathsf{T}} q_h^{(2j+1)} = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{l=1}^{2j} (-1)^{l+1} q_h^{(l)\mathsf{T}} p_h^{(2j+1-l)}\Big) \tag{27}$$

is also a total differential. We now distinguish the following situations:

Case A: both multistep methods are identical. This case has been treated in Section XV.4.3 of [10]. We have $\lambda_j^p = \lambda_j^q$ for all j, and it follows from (27) that the

entire left-hand side of (26) is a total differential. Using the modified differential equation (18), first and higher derivatives of p_h and q_h can be substituted with expressions depending only on p_h and q_h. This proves the existence of functions $H_{2j}(p,q)$, such that after integration of (26)

$$H(p_h,q_h)+h^2H_2(p_h,q_h)+h^4H_4(p_h,q_h)+\ldots = \text{const}+\mathscr{O}(th^N). \qquad (28)$$

As long as the solution of the modified differential equation (i.e., the numerical solution) remains in a compact set, we thus have $H(p_h,q_h)=\text{const}+\mathscr{O}(h^r)+\mathscr{O}(th^N)$, where r is the order of the method and N can be chosen arbitrarily large.

This is a nice result, but of limited interest. If the p and q components are discretized by the same multistep method, parasitic components are usually not under control and they destroy the long-time behavior of the underlying one-step method.

Case B: separable Hamiltonian with quadratic kinetic energy. This situation is treated in [9]. For a Hamiltonian of the form $H(p,q)=\frac{1}{2}p^{\mathsf{T}}M^{-1}p+U(q)$ (without loss of generality we assume $M=I=$identity) we have $\nabla_p H(p,q)=p$. The second relation of (24) therefore permits to express p_h as a linear combination of odd derivatives of q_h. Inserted into (26), this gives rise to a linear combination of terms $q_h^{(m)\mathsf{T}}q_h^{(2j+1-m)}$, which all can be written as total differentials because of

$$2q_h^{(m)\mathsf{T}}q_h^{(2j+1-m)}=\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{l=m}^{2j-m}(-1)^{l-m}q_h^{(l)\mathsf{T}}q_h^{(2j-l)}\Big). \qquad (29)$$

Without any assumptions on the coefficients λ_j^p and λ_j^q, a modified Hamiltonian satisfying (28) can be obtained as in Case (A). This is an important result, because the parasitic components can be shown to remain bounded and small (see [9] and Chapter 3 below).

Case C: additional order conditions. If both multistep schemes are of order r, then $\lambda_j^p=\lambda_j^q=0$ holds for $1\le j<r$. Can we construct schemes, where the polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ have no common zeros other than $\zeta=1$, such that $\lambda_j^p=\lambda_j^q$ also for $j=r$ (and possibly also for larger j)?

The class of explicit, symmetric 3-step methods of order $r=2$ is given by

$$\rho(\zeta)=(\zeta-1)(\zeta^2+2a\zeta+1),\qquad \sigma(\zeta)=(a+1)(\zeta^2+\zeta),$$

where $|a|<1$ by stability (for $a=1$ it is reducible and equivalent to the 2-step explicit midpoint rule). The coefficient λ_2 in the expansion (25) is $\lambda_2=\frac{1}{2}\big(\frac{1}{a+1}-\frac{1}{6}\big)$, and it is not possible to have the same λ_2 for different values of a.

Symmetric 5-step methods of order $r=4$ are given by

$$\rho(\zeta)=(\zeta-1)(\zeta^2+2a_1\zeta+1)(\zeta^2+2a_2\zeta+1),$$

where $|a_1|<1$ and $|a_2|<1$ (one of these coefficients is allowed to be equal to 1, but then the method reduces to a 4-stage method). The polynomial $\sigma(\zeta)$ is uniquely determined by assuming the method to be explicit and of order 4. In this case, the

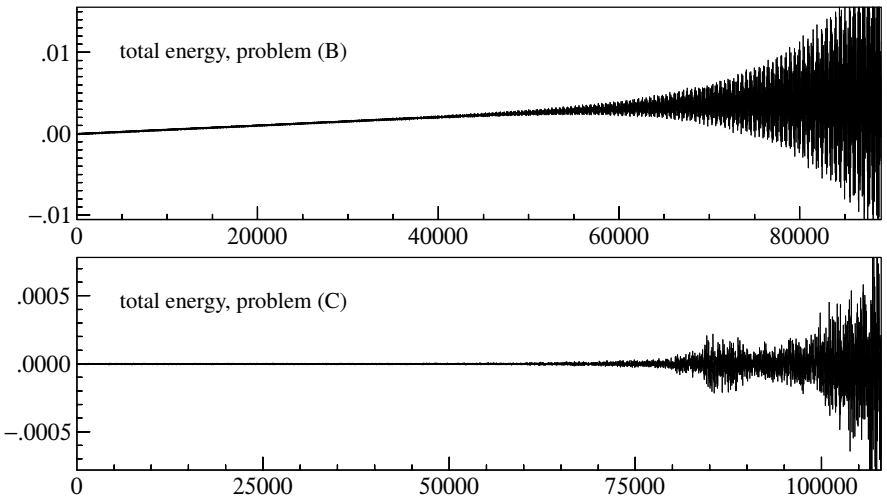


Fig. 4 Numerical Hamiltonian of method 'plmm4c' applied with step size $h = 0.005$ for problem (B), and with $h = 0.001$ for problem (C); initial values and starting approximations as in Figure 1.

coefficient

$$\lambda_4 = \frac{131 - 19\,(a_1 + a_2) + 11\,a_1 a_2}{720\,(1 + a_1)(1 + a_2)}$$

in (25) depends on two parameters, and it is possible to construct different methods with the same value of λ_4. This happens, for example, when the coefficients $a_j^p = \cos\theta_j^p$ and $a_j^q = \cos\theta_j^q$ for the two ρ polynomials are given by

$$\text{plmm4c} \qquad \begin{aligned} \rho_p(\zeta): &\quad \theta_1^p = \pi/8 \qquad \theta_2^p = 3\pi/4 \\ \rho_q(\zeta): &\quad \theta_1^q = 3\pi/8 \qquad \theta_2^q \approx 0.68\,\pi \end{aligned}$$

(here, θ_1^p, θ_2^p, θ_1^q are arbitrarily fixed, and θ_2^q is computed to satisfy $\lambda_4^p = \lambda_4^q$). We apply this method to the three problems with separable Hamiltonian of Section 1.3. For problem (A) there is no difference to the behavior of methods plmm2 and plmm4. The error in the Hamiltonian is of size $\mathcal{O}(h^4)$ and no drift can be observed. Numerical results for problems (B) and (C) are presented in Figure 4. For problem (B) we expect that the dominant error term in the Hamiltonian remains bounded. In fact, experiments with many different values of the step size h indicate that the error in the Hamiltonian is bounded by $\mathcal{O}(h^4) + \mathcal{O}(th^6)$ on intervals of length $\mathcal{O}(h^{-2})$. Similarly, also for problem (C) the dominant error term remains bounded. In this case we expect the error to behave like $\mathcal{O}(h^4) + \mathcal{O}(\sqrt{t}h^6)$. The second term is invisible on intervals of length $\mathcal{O}(h^{-2})$, see also Table 1. Beyond such an interval, Figure 4 shows that for both problems, (B) and (C), the error behaves like $\delta\exp(ch^2t)$ with a small constant δ. This undesirable exponential error growth will be explained by studying parasitic solution components in Chapter 3.

2.4 Near preservation of quadratic first integrals

We again consider general differential equations (1) and we assume the existence of a quadratic first integral of the form $L(p,q) = p^{\mathsf{T}} E\, q$, i.e.,

$$f(p,q)^{\mathsf{T}} E\, q + p^{\mathsf{T}} E\, g(p,q) = 0 \qquad \text{for all } p \text{ and } q. \tag{30}$$

The exact solution satisfies $L\big(p(t),q(t)\big) = \text{const}$, and we are interested to know if the numerical approximation can mimic this behavior. As in the previous section we consider only smooth numerical approximations, which are formally equal to the values of the solution $\big(p_h(t),q_h(t)\big)$ at $t = nh$ of the modified differential equation. We therefore have to study the evolution of $L\big(p_h(t),q_h(t)\big)$.

Dividing the relations in (20) by h times the σ polynomials, the solution of the modified differential equation is seen to verify

$$\begin{aligned} \big(1+\lambda_1^p hD+\lambda_2^p h^2D^2+\ldots\big)\dot p_h &= f(p_h,q_h)+\mathscr{O}(h^N) \\ \big(1+\lambda_1^q hD+\lambda_2^q h^2D^2+\ldots\big)\dot q_h &= g(p_h,q_h)+\mathscr{O}(h^N), \end{aligned} \tag{31}$$

where the coefficients λ_j^p and λ_j^q are given by (25). We restrict our considerations to symmetric methods, so that the series are in even powers of h. We multiply the transposed first relation of (31) with Eq_h from the right, and the second one with $p_h^{\mathsf{T}}E$ from the left, and we add both so that by (30) the right-hand side becomes an expression of size $\mathscr{O}(h^N)$. We thus obtain

$$\big((1+\lambda_2^p h^2D^2+\ldots)\dot p_h\big)^{\mathsf{T}} E\, q_h + p_h^{\mathsf{T}} E(1+\lambda_2^q h^2D^2+\ldots)\,\dot q_h = \mathscr{O}(h^N). \tag{32}$$

An important simplification can be achieved by using the identity

$$(p_h^{2j+1})^{\mathsf{T}} E\, q_h + p_h^{\mathsf{T}} E\, q_h^{(2j+1)} = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{l=0}^{2j}(-1)^l (p_h^{(2j-l)})^{\mathsf{T}} E\, q_h^{(l)}\Big) \tag{33}$$

As in the previous section we now distinguish the following situations:

Case A: both multistep methods are identical. This is the case considered in Section XV.4.4 of [10]. We have $\lambda_j^p = \lambda_j^q$ for all j, and it follows from (33) that the expression in (32) is a total differential. As in Section 2.3, first and higher derivatives of p_h and q_h can be substituted with expressions depending only on p_h and q_h. Hence, there exist functions $L_{2j}(p,q)$ with $L_0(p,q) = L(p,q) = p^{\mathsf{T}} E\, q$, such that after integration of (32)

$$L(p_h,q_h) + h^2 L_2(p_h,q_h) + h^4 L_4(p_h,q_h) + \ldots = \text{const} + \mathscr{O}(th^N). \tag{34}$$

As long as the solution of the modified differential equation (i.e., the numerical solution) remains in a compact set, we thus have $L(p_h,q_h) = \text{const} + \mathscr{O}(h^r) + \mathscr{O}(th^N)$, where r is the order of the method and N can be chosen arbitrarily large.

Note that such a result is not true in general for symmetric one-step methods. However, it is of limited interest, because parasitic components are usually not under control for the situation, where both multistep methods are identical.

Case B: special form of the differential equation. We consider problems of the form

$$\dot{p} = f(q), \qquad \dot{q} = M^{-1} p,$$

which are equivalent to second order differential equations $\ddot{q} = M^{-1} f(q)$. This corresponds to the situation treated in [9]. Without loss of generality we assume in the following that $M = I =$identity). For such special differential equations the condition (30) splits into two conditions

$$f(q)^{\mathsf{T}} E\, q = 0, \qquad p^{\mathsf{T}} E\, p = 0 \qquad \text{for all } p \text{ and } q,$$

which implies that E is a skew-symmetric matrix. Moreover, because of $g(p,q) = p$, the second relation of (31) permits to express p_h as a linear combination of odd derivatives of q_h. Inserted into (32), this gives rise to a linear combination of terms $q_h^{(2m+1)\mathsf{T}} E\, q_h^{(2j-2m+1)}$, which can be written as total differentials because

$$q_h^{(2m+1)\mathsf{T}} E\, q_h^{(2j-2m+1)} = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{l=2m+1}^{j} (-1)^{l-1} q_h^{(l)\mathsf{T}} E\, q_h^{(2j-l+1)} \Big).$$

Without any assumptions on the coefficients λ_j^p and λ_j^q, a formal first integral of the form (34) is obtained that is $\mathcal{O}(h^r)$-close to the invariant $L(p,q) = p^{\mathsf{T}} E\, q$ of the differential equation. This result is important, because the parasitic components will be shown to remain bounded and small (see also [9]).

Case C: additional order conditions. If the partitioned multistep method is of order r, we have $\lambda_j^p = \lambda_j^q = 0$ for $1 \le j < r$. If the coefficients of the method are constructed such that $\lambda_j^p = \lambda_j^q$ also for $j = r$, we can apply the computation of case (A) to the leading error term. In this way an improved near conservation of quadratic first integrals can be achieved, similar to the near energy conservation in the previous section.

2.5 Symplecticity and conjugate symplecticity

In the numerical solution of Hamiltonian systems it is unavoidable to speak also about symplecticity. Together with the differential equation

$$\begin{aligned} \dot{p} &= -\nabla_q H(p,q), \\ \dot{q} &= \nabla_p H(p,q), \end{aligned} \tag{35}$$

whose flow we denote by $\varphi_t(p_0, q_0)$, we consider the variational differential equation

$$\begin{aligned} \dot P &= -\nabla^2_{qp} H(p,q)\, P - \nabla^2_{qq} H(p,q)\, Q, \\ \dot Q &= \quad \nabla^2_{pp} H(p,q)\, P + \nabla^2_{pq} H(p,q)\, Q, \end{aligned} \tag{36}$$

where we use the notation $\nabla^2_{qp} H(p,q) = \big(\frac{\partial^2 H}{\partial q_i \partial p_j}\big)$. Here, $P(t)$ and $Q(t)$ are the derivatives with respect to initial values,

$$P(t) = \Big(\frac{\partial p(t)}{\partial p_0}, \frac{\partial p(t)}{\partial q_0}\Big), \quad Q(t) = \Big(\frac{\partial q(t)}{\partial p_0}, \frac{\partial q(t)}{\partial q_0}\Big) \quad \text{and} \quad \varphi'_t(p_0,q_0) = \begin{pmatrix} P(t) \\ Q(t) \end{pmatrix}.$$

The flow map $\varphi_t(p_0,q_0)$ of (35) is a symplectic transformation, see e.g., [10, VI.2]. This means, by definition, that its Jacobian matrix satisfies

$$\varphi'_t(p_0,q_0)^{\mathsf T} J\, \varphi'_t(p_0,q_0) = J \quad \text{or equivalently} \quad P(t)^{\mathsf T} Q(t) - Q(t)^{\mathsf T} P(t) = J,$$

where J is the canonical structure matrix already encountered in (16). The important observation is that symplecticity just means that $P^{\mathsf T} Q - Q^{\mathsf T} P$ is a quadratic first integral of the combined system (35)-(36).

The smooth numerical solution of a partitioned multistep method is formally equal to the exact solution of the modified differential equation of Theorem 1. We therefore call the multistep method *symplectic*, if the derivative $(P_h(t), Q_h(t))$ (with respect to initial values) of the solution $(p_h(t), q_h(t))$ of the modified differential equation (18) satisfies

$$P_h(t)^{\mathsf T} Q_h(t) - Q_h(t)^{\mathsf T} P_h(t) = J.$$

Unfortunately, this is never satisfied unless for some trivial exceptions (implicit midpoint rule, symplectic Euler method, and the Störmer–Verlet scheme) which are partitioned linear multistep methods and one-step methods at the same time. Intuitively this is clear from the considerations of Section 2.4, because we did not encounter any result on the exact preservation of quadratic first integrals. A rigorous proof of this negative result has first been given by Tang [17] (see also [10, Sect. XV.4]).

In view of this negative result, it is natural to consider a weaker property than symplecticity, which nevertheless retains the same qualitative long-time behavior. We call a matrix-valued mapping $\Phi_h : (p,q) \mapsto (P,Q)$ *conjugate symplectic*, if there exists a global change of coordinates $(\widehat p, \widehat q) = \chi_h(p,q)$ that is $\mathscr{O}(h^r)$-close to the identity, such that the mapping is symplectic in the new coordinates, i.e., the mapping $\widehat\Phi_h = \chi_h \circ \Phi_h \circ \chi_h^{-1}$ is a symplectic transformation. Since

$$\widehat\Phi'_h(\widehat p, \widehat q) = \Phi'_h(p,q) + h^r K_r(p,q) + h^{r+1} K_{r+1}(p,q) + \ldots,$$

the symplecticity of $\widehat\Phi_h$ yields the existence of functions $L_j(p,q)$ such that

$$\Phi'_h(p,q)^{\mathsf T} J\, \Phi'_h(p,q) + h^r L_r(p,q) + h^{r+1} L_{r+1}(p,q) + \ldots = J. \tag{37}$$

This means that for a method that is conjugate symplectic, there exists a modified first integral (as a formal series in powers of h) of the modified differential equation which is $\mathscr{O}(h^r)$-close to $P_h^{\mathsf{T}} Q_h - Q_h^{\mathsf{T}} P_h = (\Phi_h')^{\mathsf{T}} J \Phi_h'$.

If Φ_h represents the underlying one-step method of a partitioned multistep method, we know from Section 2.4 that under suitable assumptions there exist functions $L_j(p,q)$ such that (37) holds. Does this imply that the method Φ_h is conjugate symplectic? That this is indeed the case follows from results of Chartier, Faou, and Murua [4], see also [10, Section XV.4.4]. We do not pursue this question in the present work.

3 Long-term stability of parasitic solution components

We consider the partitioned linear multistep method (2) applied to the differential equation (1). We assume that both multistep methods are symmetric and stable, so that the zeros of the polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ are all on the unit circle. We denote these zeros by $\zeta_0 = 1$, and ζ_j, $\zeta_{-j} = \overline{\zeta}_j$ for $j = 1, \ldots, \kappa$ (if -1 is such a zero, we let $\zeta_{-\kappa} = \zeta_\kappa = -1$). Furthermore, we consider finite products of the zeros of the ρ-polynomials, which we again denote by ζ_j and $\zeta_{-j} = \overline{\zeta}_j$. The resulting index set is denoted by $\mathscr{I}$, so that

$$\{\zeta_l\}_{l \in \mathscr{I}} = \{\zeta = \zeta_1^{m_1} \cdot \ldots \cdot \zeta_\kappa^{m_\kappa};\ m_j \geq 0\}.$$

The index set can be finite (if all zeros of the ρ-polynomials are roots of unity) or it can be infinite. It is convenient to denote $\mathscr{I}^* = \mathscr{I} \setminus \{0\}$.

Our aim is to write the numerical solution of (2) in the form

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = \begin{pmatrix} p(t_n) \\ q(t_n) \end{pmatrix} + \sum_{l \in \mathscr{I}^*} \zeta_l^n \begin{pmatrix} u_l(t_n) \\ v_l(t_n) \end{pmatrix}, \tag{38}$$

where $t_n = nh$. Here, $(p(t), q(t))$ is an h-dependent approximation to the exact solution of (1), called *principal solution component*. To avoid any confusion, we denote in this chapter the exact solution of (1) as $(p_{exact}(t), q_{exact}(t))$. The functions $(u_l(t), v_l(t))$ also depend on the step size h, and they are called *parasitic solution components*. This chapter is devoted to get bounds on these parasitic solution components and to investigate the length of time intervals, where the parasitic components do not significantly perturb the principal solution component.

A similar representation of the numerical solution has been encountered when discussing the numerical solution for the harmonic oscillator in Section 2.1. There, only zeros of the ρ-polynomials are present in the sum. The appearance of products of such zeros in (38) is due to the nonlinearity of the vector field in (1).

3.1 Modified differential equation (full system)

We first study the existence of the coefficient functions in the representation (38). This is an extension of the backward error analysis of the smooth numerical solution as discussed in Section 2.2. It follows closely the presentation of [10, Sect. XV.3.2]. In the following we use the notations $y(t) = (p(t), q(t))$, $z_l(t) = (u_l(t), v_l(t))$, and we collect in the vector $\mathbf{z}(t)$ the components $u_l(t)$ ($l \neq 0$) for which $\rho_p(\zeta_l) = 0$ and the components $v_l(t)$ ($l \neq 0$) for which $\rho_q(\zeta_l) = 0$.

Theorem 2. *Consider a consistent, symmetric, partitioned linear multistep method (2), applied to the differential equation (1). Then, there exist h-independent functions $f_j(p,q,\mathbf{z})$, $g_j(p,q,\mathbf{z})$, and $f_{l,j}(p,q,\mathbf{z})$, $g_{l,j}(p,q,\mathbf{z})$, such that for an arbitrarily chosen truncation index N and for every solution $p(t), q(t), u_l(t), v_l(t)$ of the system*

$$\begin{aligned}
\dot p &= f(p,q) + hf_1(p,q,\mathbf{z}) + \ldots + h^{N-1} f_{N-1}(p,q,\mathbf{z}) \\
\dot q &= g(p,q) + hg_1(p,q,\mathbf{z}) + \ldots + h^{N-1} g_{N-1}(p,q,\mathbf{z}) \\
\dot u_l &= f_{l,0}(p,q,\mathbf{z}) + hf_{l,1}(p,q,\mathbf{z}) + \ldots + h^{N-1} f_{l,N-1}(p,q,\mathbf{z}) \qquad \text{if} \quad \rho_p(\zeta_l) = 0 \\
\dot v_l &= g_{l,0}(p,q,\mathbf{z}) + hg_{l,1}(p,q,\mathbf{z}) + \ldots + h^{N-1} g_{l,N-1}(p,q,\mathbf{z}) \qquad \text{if} \quad \rho_q(\zeta_l) = 0 \\
u_l &= hf_{l,1}(p,q,\mathbf{z}) + \ldots + h^N f_{l,N}(p,q,\mathbf{z}) \qquad \text{if} \quad \rho_p(\zeta_l) \neq 0 \\
v_l &= hg_{l,1}(p,q,\mathbf{z}) + \ldots + h^N g_{l,N}(p,q,\mathbf{z}) \qquad \text{if} \quad \rho_q(\zeta_l) \neq 0 \\
u_l &= 0, \;\; v_l = 0 \qquad \text{if} \quad \zeta_l \neq \zeta_1^{m_1} \cdot \ldots \cdot \zeta_\kappa^{m_\kappa} \;\; \text{with} \;\; m_1 + \ldots + m_\kappa < N,
\end{aligned} \tag{39}$$

with initial values $\mathbf{z}(0) = \mathscr{O}(h)$, the function (with $n = t/h$)

$$\begin{pmatrix} p_h(t) \\ q_h(t) \end{pmatrix} = \begin{pmatrix} p(t) \\ q(t) \end{pmatrix} + \sum_{l \in \mathscr{I}^*} \zeta_l^n \begin{pmatrix} u_l(t) \\ v_l(t) \end{pmatrix}, \tag{40}$$

satisfies the multistep formula up to a defect of size $\mathscr{O}(h^{N+1})$, i.e.,

$$\begin{aligned}
\sum_{j=0}^{k} \alpha_j^p \, p_h(t+jh) &= h \sum_{j=0}^{k} \beta_j^p \, f\big(p_h(t+jh), q_h(t+jh)\big) + \mathscr{O}(h^{N+1}) \\
\sum_{j=0}^{k} \alpha_j^q \, q_h(t+jh) &= h \sum_{j=0}^{k} \beta_j^q \, g\big(p_h(t+jh), q_h(t+jh)\big) + \mathscr{O}(h^{N+1})
\end{aligned} \tag{41}$$

as long as $(p(t), q(t))$ remain in a compact set, and $\|\mathbf{z}(t)\| \leq Ch$. The constant symbolized by $\mathscr{O}$ is independent of h, but depends on the truncation index N. It also depends smoothly on t. If the partitioned multistep method is of order r, then we have $f_l(p,q) = g_l(p,q) = 0$ for $1 \leq l < r$.

Remark 2. Because of the last line in (39), the sum in (40) is always finite. Substituting $\mathbf{z} = 0$ in the upper two equations of (39) yields the modified differential equation (18) of Section 2.2. The solution of the system (39) satisfies $u_{-l}(t) = \overline{u}_l(t)$, $v_{-l}(t) = \overline{v}_l(t)$, whenever these relations hold for the initial values.

Proof. The proof is very similar to that of Theorem 1, and we highlight here only the main differences. We insert the finite sum (40) into (41), we expand the nonlinearities around $(p(t),q(t))$, which we also denote by $(u_0(t),v_0(t))$, and we compare the coefficients of ζ_j^n. This yields, recalling that $y(t)=(p(t),q(t))=(u_0(t),v_0(t))$ and $z_l(t)=(u_l(t),v_l(t))$, and omitting the argument t,

$$\begin{aligned}
\rho_p(\zeta_l \mathrm{e}^{hD})u_l &= h\,\sigma_p(\zeta_l \mathrm{e}^{hD}) \sum_{m\ge 0} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} f^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}),\\
\rho_q(\zeta_l \mathrm{e}^{hD})v_l &= h\,\sigma_q(\zeta_l \mathrm{e}^{hD}) \sum_{m\ge 0} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} g^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}),
\end{aligned} \tag{42}$$

where the second sum is over indices $l_1\neq 0,\ldots,l_m\neq 0$. The summand for $m=0$, which is $f(y(t))$, resp. $g(y(t))$, is present only for $l=0$, i.e., for $\zeta_l=1$. Notice further that for $l=0$ the summand for $m=1$ vanishes, because we always have $\zeta_{l_1}\neq\zeta_0$. In view of an inversion of the operators $\rho_p(\zeta_l \mathrm{e}^{hD})$ and $\rho_q(\zeta_l \mathrm{e}^{hD})$ we introduce the coefficients of the expansions (cf. equation (21) for $\zeta_0=1$)

$$\frac{x\,\sigma_p(\zeta_l\,\mathrm{e}^x)}{\rho_p(\zeta_l\,\mathrm{e}^x)} = \mu_{l0}^p + \mu_{l1}^p x + \mu_{l2}^p x^2 + \ldots, \quad \frac{x\,\sigma_q(\zeta_l\,\mathrm{e}^x)}{\rho_q(\zeta_l\,\mathrm{e}^x)} = \mu_{l0}^q + \mu_{l1}^q x + \mu_{l2}^q x^2 + \ldots\,. \tag{43}$$

If $\rho_p(\zeta_l)\neq 0$, we have $\mu_{l0}^p=0$. If $\rho_p(\zeta_l)=0$, the expansion exists because ζ_l is a simple zero, and we have $\mu_{l0}^p\neq 0$ because $\sigma_p(\zeta_l)\neq 0$ as a consequence of the irreducibility of the method. The same statements hold for the second method. We therefore obtain the differential equations

$$\begin{aligned}
\dot u_l &= \big(\mu_{l0}^p + \mu_{l1}^p hD + \ldots\big) \sum_{m\ge 0} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} f^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^N), \\
&\qquad\qquad \text{if } \rho_p(\zeta_l)=0,\\
\dot v_l &= \big(\mu_{l0}^q + \mu_{l1}^q hD + \ldots\big) \sum_{m\ge 0} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} g^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^N), \\
&\qquad\qquad \text{if } \rho_q(\zeta_l)=0,
\end{aligned} \tag{44}$$

and the algebraic relations

$$\begin{aligned}
u_l &= \big(\mu_{l1}^p hD + \mu_{l2}^p h^2D^2 + \ldots\big) \sum_{m\ge 1} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} f^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}), \\
&\qquad\qquad \text{if } \rho_p(\zeta_l)\neq 0,\\
v_l &= \big(\mu_{l1}^q hD + \mu_{l2}^q h^2D^2 + \ldots\big) \sum_{m\ge 1} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} g^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}), \\
&\qquad\qquad \text{if } \rho_q(\zeta_l)\neq 0.
\end{aligned} \tag{45}$$

As in the proof of Theorem 1 we use (44) to recursively eliminate first and higher derivatives of u_l if $\rho_p(\zeta_l)=0$ and of v_l if $\rho_q(\zeta_l)=0$. Similarly, we use (45) to recursively eliminate u_l and its derivatives if $\rho_p(\zeta_l)\neq 0$ and of v_l and its derivatives if

$\rho_q(\zeta_l) \neq 0$. Collecting equal powers of h yields the functions $f_j(p,q,\mathbf{z})$, $g_j(p,q,\mathbf{z})$, and $f_{l,j}(p,q,\mathbf{z})$, $g_{l,j}(p,q,\mathbf{z})$.

If $\zeta_l \neq \zeta_1^{m_1} \cdots \zeta_\kappa^{m_\kappa}$ with $m_1 + \ldots + m_\kappa < N$, the right-hand side of (45) contains at least N factors of components of $\mathbf{z}$. By our assumption $\|\mathbf{z}(t)\| \leq Ch$, this implies $u_l = \mathscr{O}(h^{N+1})$ and $v_l = \mathscr{O}(h^{N+1})$, so that these functions can be included in the remainder term. This justifies the last line of (39) and concludes the proof of the theorem. □

Initial values for the system (39). For an application of the multistep formula (2), starting approximations (p_j, q_j) for $j = 0, \ldots, k-1$ have to be provided. We assume that they satisfy (with $0 \leq \nu \leq r$)

$$p_j - p_{exact}(jh) = \mathscr{O}(h^{\nu+1}), \quad q_j - q_{exact}(jh) = \mathscr{O}(h^{\nu+1}), \quad j = 0, \ldots, k-1. \tag{46}$$

Initial values for the differential equation (39) have to be such that

$$\begin{pmatrix} p_j \\ q_j \end{pmatrix} = \begin{pmatrix} p(jh) \\ q(jh) \end{pmatrix} + \sum_{l \in \mathscr{J}^*} \zeta_l^j \begin{pmatrix} u_l(jh) \\ v_l(jh) \end{pmatrix}, \qquad j = 0, \ldots, k-1. \tag{47}$$

The solution of (39) is uniquely determined by the initial values $y(0), \mathbf{z}(0)$ (for the notation of y and $\mathbf{z}$ see the beginning of Section 3.1), so that the system (47) can be written as $F\big(y(0), \mathbf{z}(0), h\big) = 0$. For $h = 0$, it represents a linear Vandermonde system for $y(0), \mathbf{z}(0)$, which gives a unique solution. The Implicit Function Theorem thus proves the local existence of a solution of $F\big(y(0), \mathbf{z}(0), h\big) = 0$ for sufficiently small step sizes h. Note that the initial values depend smoothly on h. Under the assumption (46) we have $p(0) = p_{exact}(0) + \mathscr{O}(h^{\nu+1})$, $q(0) = q_{exact}(0) + \mathscr{O}(h^{\nu+1})$, and $\mathbf{z}(0) = \mathscr{O}(h^{\nu+1})$.

3.2 Growth parameters

Before attacking the question of bounding rigorously the parasitic solution components, we try to get a feeling of the solution of the system (39). This system is equivalent to the equations (44) and (45). Our aim is to have small parasitic solution components. We therefore neglect all terms that are at least quadratic in $\mathbf{z}$.

The equations (44) for $l = 0$ (principal solution components) become equivalent to the modified equation already studied in Chapter 2. If we consider only the leading (h-independent) term in the expansion (45), we get zero functions. All that remains are the equations (44) with $l \neq 0$ which, for $h = 0$, are as follows:

- if ζ_l is a common zero of $\rho_p(\zeta)$ and $\rho_q(\zeta)$, we have

$$\begin{aligned} \dot{u}_l &= \mu_{l0}^p \big(f_p(p(t),q(t))\, u_l + f_q(p(t),q(t))\, v_l \big) \\ \dot{v}_l &= \mu_{l0}^q \big(g_p(p(t),q(t))\, u_l + g_q(p(t),q(t))\, v_l \big), \end{aligned} \tag{48}$$

- if ζ_l is a zero of $\rho_p(\zeta)$, but $\rho_q(\zeta_l) \neq 0$, we have

$$\dot{u}_l = \mu_{l0}^p f_p(p(t),q(t))\, u_l, \tag{49}$$

- if ζ_l is a zero of $\rho_q(\zeta)$, but $\rho_p(\zeta_l) \neq 0$, we have

$$\dot{v}_l = \mu_{l0}^q g_q(p(t),q(t))\, v_l. \tag{50}$$

The coefficient $\mu_l = \mu_{l0}$ is called *growth parameter* of a multistep method with generating polynomials $\rho(\zeta)$ and $\sigma(\zeta)$. It is defined by (43) for the limit $x \to 0$, and can be computed from

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

We remark that for a symmetric linear multistep method the growth parameter is always real. This follows from $\sigma(1/\zeta_l) = \zeta_l^k \sigma(\zeta_l)$ and $-\zeta_l^{-2}\rho'(\zeta_l) = \zeta_l^k \rho'(\zeta_l)$, which is obtained by differentiation of the relation $\rho(1/\zeta) = \zeta^k \rho(\zeta)$.

Already when we use for $(p(t),q(t))$ the exact solution of the original problem, the equations (48)-(50) give much insight into the behavior of the multistep method. For example, if we consider the harmonic oscillator, for which $f(p,q) = -q$, $g(p,q) = p$, the differential equation (48) gives bounded solutions only if the product of the growth parameters of both methods satisfy $\mu_l^p \mu_l^q > 0$ for all l. For nonlinear problems, the differential equation (48) has bounded solutions only in very exceptional cases.

If the polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ do not have common zeros with the exception of $\zeta_0 = 1$, the situation with equation (48) cannot arise. Therefore, only the equations (49) and (50) are relevant. There are many interesting situations, where tthe solutions of these equations are bounded, e.g., if $f(p,q)$ only depends on q and $g(p,q)$ only depends on p, what is the case for Hamiltonian systems with separable Hamiltonian.

3.3 Bounds for the parasitic solution components

We study the system (39) of modified differential equations. We continue to use the notation $y = (p,q)$ and, as in Section 3.1, we denote by $\mathbf{z}(t)$ the vector whose components are $u_l(t)$ ($l \neq 0$) for which $\rho_p(\zeta_l) = 0$ and $v_l(t)$ ($l \neq 0$) for which $\rho_q(\zeta_l) = 0$. The system (39) can then be written in compact notations as

$$\begin{aligned} \dot{y} &= F_{h,N}(y) + G_{h,N}(y,\mathbf{z}) \\ \dot{\mathbf{z}} &= A_{h,N}(y)\,\mathbf{z} + B_{h,N}(y,\mathbf{z}), \end{aligned} \tag{51}$$

where $G_{h,N}(y,\mathbf{z})$ and $B_{h,N}(y,\mathbf{z})$ collect those terms that are quadratic or of higher order in $\mathbf{z}$. Note that, by the construction via the system (44), the differential equation for y does not contain any linear term in $\mathbf{z}$.

We consider a compact subset K_0 of the $y = (p,q)$ phase space, and for a small positive parameter δ we define

$$K = \big\{ (y,\mathbf{z}) \, ; \, y \in K_0, \|\mathbf{z}\| \le \delta \big\}. \tag{52}$$

Regularity of the (original) differential equation implies that there exists a constant L such that

$$\|G_{h,N}(y,\mathbf{z})\| \le L\,\|\mathbf{z}\|^2, \qquad \|B_{h,N}(y,\mathbf{z})\| \le L\,\|\mathbf{z}\|^2 \qquad \text{for} \quad (y,\mathbf{z}) \in K. \tag{53}$$

Our aim is to get bounds on the parasitic solution components $\mathbf{z}(t)$, which then allow to get information on the long-time behavior of partitioned linear multistep methods. To this end, we consider the simplified system

$$\begin{aligned} \dot{y} &= F_{h,N}(y), \\ \dot{\mathbf{z}} &= A_{h,N}(y)\,\mathbf{z}, \end{aligned} \tag{54}$$

where quadratic and higher order terms of $\mathbf{z}$ have been removed from (51). The differential equation for y is precisely the modified differential equation for the smooth numerical solution (Section 2.2). The differential equation for $\mathbf{z}$ is linear with coefficients depending on time t through the solution $y(t)$. Its dominant h-independent term is the differential equation studied in Section 3.2.

In the case of linear multistep methods for second order Hamiltonian systems, a formal invariant of the full system (51) has been found that is close to $\|\mathbf{z}\|$ (see [9] or [10, Sect. XV.5.3]; the ideas are closely connected to the study of adiabatic invariants in highly oscillatory differential equations [8]). This was the key for getting bounds of the parasitic solution components on time intervals that are much longer than the natural time scale of the system (54). Here, we include the existence of such a formal invariant in an assumption ('S' for stability and 'I' for invariant), and we later discuss situations, where it is satisfied.

Stability assumption (SI). *We say that a partitioned linear multistep method (2) applied to a partitioned differential equation (1) satisfies the stability assumption (SI), if there exists a smooth function $I_{h,N}(y,\mathbf{z})$ such that, for $0 < h \le h_0$,*

- *the invariance property*

$$I_{h,N}\big(y(h),\mathbf{z}(h)\big) = I_{h,N}\big(y(0),\mathbf{z}(0)\big) + \mathcal{O}(h^{M+1}\|z(0)\|^2)$$

  holds for solutions of the differential equation (54), for which $(y(t),\mathbf{z}(t)) \in K$ for t in the interval $0 \le t \le h$;
- *there exists a constant $C \ge 1$, such that*

$$I_{h,N}(y,\mathbf{z}) \le \|\mathbf{z}\|^2 \le C\,I_{h,N}(y,\mathbf{z}) \quad \textit{for} \quad (y,\mathbf{z}) \in K.$$

We are interested in situations, where the stability assumption (SI) is satisfied with $M > 0$, and we obviously focus on situations which admit a large M.

Lemma 1. *Under the stability assumption (SI) we have, for* $0 < h \le h_0$*,*

$$I_{h,N}\big(y(h),\mathbf{z}(h)\big) = I_{h,N}\big(y(0),\mathbf{z}(0)\big) + \mathscr{O}(h^{M+1}\|\mathbf{z}(0)\|^2) + \mathscr{O}(h\,\delta\|\mathbf{z}(0)\|^2)$$

along solutions of the complete system (51) of modified differential equations, provided that they stay in the compact set K for $0 \le t \le h$*.*

Proof. The defect of the solution $(y(t),\mathbf{z}(t))$ of (51), when inserted into (54), is bounded by $\mathscr{O}(\|\mathbf{z}(0)\|^2)$. An application of the Gronwall Lemma therefore proves that the difference of the solutions of the two systems with identical initial values is bounded by $\mathscr{O}(h\|\mathbf{z}(0)\|^2)$. The statement then follows from the mean value theorem applied to the function $I_{h,N}(y,\mathbf{z})$ and from the fact that the derivative still contains a factor of $\mathbf{z}$. □

We are now able to state and prove the main result of this chapter. It tells us the length of the integration interval, on which the parasitic solution components do not destroy the long-time behavior of the underlying one-step method.

Theorem 3. *In addition to the stability assumption (SI) we require that*

(A1) the partitioned linear multistep method (2) is symmetric, of order r, and the generating polynomials $\rho_p(\zeta)$ *and* $\rho_q(\zeta)$ *do not have common zeros with the exception of* $\zeta = 1$*;*

(A2) the vector field of (1) is defined and analytic in an open neighborhood of a compact set K_1*;*

(A3) the numerical solution $y_n = (p_n, q_n)$ *stays for all n with* $0 \le nh \le T_0$ *in a compact set* $K_0 \subset K_1$ *which has positive distance from the boundary of* K_1*;*

(A4) the starting approximations (p_j, q_j), $j = 0,\dots,k-1$ *are such that the initial values for the full modified differential equation (51) satisfy* $y(0) \in K_0$*, and* $\|\mathbf{z}(0)\| \le \delta/\sqrt{2\mathrm{e}C}$ *with C from the stability assumption (SI) and* $\delta = \mathscr{O}(h)$*.*

For sufficiently small h and δ *and for a fixed truncation index N, chosen large enough such that* $h^N \le \max(h^M\delta, \delta^2)$*, there exist constants* c_1, c_2 *and functions* $y(t), z_l(t)$ *on an interval of length*

$$T = \min\big(T_0,\, c_1\,\delta^{-1},\, c_2\,h^{-M}\big), \tag{55}$$

such that

- *the numerical solution satisfies* $y_n = y(nh) + \sum_{l\in\mathscr{I}^*} \zeta_l^n\, z_l(nh)$ *for* $0 \le nh \le T$*;*
- *on every subinterval* $[mh,(m+1)h)$*, the functions* $y(t), z_l(t)$ *are a solution of the system (51);*
- *at the time instants* $t_m = mh$ *the functions* $y(t), z_l(t)$ *have jump discontinuities of size* $O(h^{N+1})$*;*
- *the parasitic solution components are bounded:* $\|\mathbf{z}(t)\| \le \delta$ *for* $0 \le nh \le T$*.*

Proof. The proof closely follows that of Theorem 8 in the publication [9], see also [10, Sect. XV.5.3]. We separate the integration interval into subintervals of length h. On a subinterval $[mh,(m+1)h)$ we define the functions $y(t) = (p(t), q(t))$

and $z_l(t) = (u_l(t), v_l(t))$ as the solution of the system (39) with initial values such that (47) holds with $j = m, m+1, \ldots, m+k-1$. It follows from Theorem 2, formula (41), that $y_{m+k} - y(t_{m+k}) = \mathcal{O}(h^{N+1})$. Consequently, the construction of initial values for the next subinterval $[(m+1)h, (m+2)h)$ yields for the functions $y(t)$ and $z_l(t)$ a jump discontinuity at t_{m+1} that is bounded by $\mathcal{O}(h^{N+1})$.

We now study how well the expression $I_{h,N}(y(t), \mathbf{z}(t))$ is preserved on long time intervals. Lemma 1 gives a bound on the maximal deviation within a subinterval of length h. Together with the $\mathcal{O}(h^{N+1})$ bound on the jump discontinuities at t_m this proves for $I_m = I_{h,N}(y(t_m), \mathbf{z}(t_m))$ the estimate

$$I_{m+1} = I_m\big(1 + C_1 h^{M+1} + C_2 h\,\delta\big) + C_3 h^{N+1}\,\delta$$

as long as $(y(t), \mathbf{z}(t))$ remains in K. With $\gamma = C_1 h^M + C_2\delta$ the discrete Gronwall Lemma thus yields

$$I_m = I_0(1+\gamma h)^m + \frac{(1+\gamma h)^m - 1}{\gamma h}\, C_3 h^{N+1}\,\delta,$$

which, for $\gamma t_m \le 1$, gives the estimate $I_m \le I_0\,\mathrm{e} + C_3(\mathrm{e}-1)h^N\delta\, t_m$. This implies

$$\|\mathbf{z}(t)\|^2 \le C\,\mathrm{e}\,\|\mathbf{z}(0)\|^2 + C_4 h^N \delta\, t,$$

so that $\|\mathbf{z}(t)\| \le \delta$ for times t subject to $\gamma t \le 1$, if the truncation index N is chosen sufficiently large. □

It is straight-forward to construct partitioned linear multistep methods of high order satisfying (A1). The assumption (A2) is satisfied for many important differential equations. The assumption (A3) can be checked a posteriori. If the method is of order r and if the starting approximations are computed with very high precision, then assumption (A4) is fulfilled with $\delta = \mathcal{O}(h^{r+1})$. This follows from the construction of the initial values for the system (39) as explained in the end of Section 3.1. The difficult task is the verification of the stability assumption (SI).

3.4 Near energy conservation

Combining our results on the long-time behavior of smooth numerical solutions with the bounded-ness of parasitic solution components we obtain the desired statements on the preservation of energy and of quadratic first integrals.

The near energy preservation has been studied analytically in Section 2.3 for smooth numerical solutions of symmetric partitioned multistep methods. We consider methods which, when applied to Hamiltonian systems, have a modified energy

$$H_h(p,q) = H(p,q) + h^r H_r(p,q) + \ldots + h^{N-1} H_{N-1}(p,q), \tag{56}$$

where r is the order of the method and $N > r$, such that

$$H_h(p_h, q_h) = \text{const} + \mathcal{O}(t\, h^N) \tag{57}$$

along solutions of the modified differential equation (18). There are situations (cases (A) and (B) of Section 2.3), where N is arbitrarily large. This is the best behavior we can hope for. In the case (C) of Section 2.3 we achieve $N = r + 2$. The worst behavior is when $N = r$, in which case a linear drift for the numerical Hamiltonian is present from the beginning. This behavior of smooth numerical solutions carries over to the general situations as follows:

Theorem 4. *Consider a partitioned linear multistep method (2) of order r, applied to a Hamiltonian system (23). Assume that there exists a modified energy (56) such that (57) holds for smooth numerical solutions.*

Under the assumptions of Theorem 3 with $\delta = \mathcal{O}(h^r)$, the numerical solution satisfies

$$H(p_n, q_n) = \text{const} + \mathcal{O}(h^r) \qquad \textit{for} \qquad nh \le T,$$

where the length of the time interval T is limited by (55) and by $T \le \mathcal{O}(h^{r-N})$.

Proof. Let $y(t) = (p(t), q(t))$ and $z_l(t)$ (for $t_m \le t \le t_{m+1}$, $t_m = mh$) be a solution of the complete system (51) as in the statement of Theorem 3. Applying the proof of Lemma 1 to the near invariant $H_h(p,q)$ yields

$$H_h\big(p(t_{m+1}), q(t_{m+1})\big) = H_h\big(p(t_m), q(t_m)\big) + \mathcal{O}(h\delta^2) + \mathcal{O}(h^{N+1}).$$

Since the jump discontinuities at the grid points t_m can be neglected, we obtain by following the proof of Theorem 3 that

$$H_h(p_n, q_n) = H_h(p_0, q_0) + \mathcal{O}(t_n \delta^2) + \mathcal{O}(t_n h^N),$$

so that the statement follows from (56) and the requirement $\delta = \mathcal{O}(h^r)$. □

Analogous statements are obtained for the near conservation of quadratic first integrals. In this case the results of Section 2.4 have to be combined with the boundedness of the parasitic solution components (Theorem 3).

3.5 Verification of the stability assumption (SI)

It remains to study the stability assumption (SI), and to investigate how large the number M in the invariance property can be. The nice feature is that we only have to consider the simplified system (54), where the subsystem for the principle solution component y is separated from the parasitic solution components. Therefore, the differential equation for $\mathbf{z}$ is a linear differential equation with coefficients depending on t via the principle solution $y(t)$. Another nice feature is that we are concerned only with a local result (estimates on an interval of length h which is the step size of the integrator).

The linear system $\dot{\mathbf{z}} = A_{h,N}(y(t))\,\mathbf{z}$ is obtained from (42), where terms are neglected that are either at least quadratic in $\mathbf{z}$ or contain a sufficiently high power of h. We consider $\zeta_l \neq 1$ satisfying $\rho_p(\zeta_l) = 0$ and $\rho_q(\zeta_l) \neq 0$. By irreducibility of the method we then have $\sigma_p(\zeta_l) \neq 0$. For ease of presentation, we assume[3] that also $\sigma_q(\zeta_l) \neq 0$. We then can apply the inverse of the operators $\sigma_p(\zeta_l \mathrm{e}^{hD})$ and $\sigma_q(\zeta_l \mathrm{e}^{hD})$ to both sides of (42) and thus obtain

$$\begin{aligned}
\Big(\frac{\rho_p}{\sigma_p}\Big)\big(\zeta_l \mathrm{e}^{hD}\big) u_l &= h \sum_{m\geq 1} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} f^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}),\\
\Big(\frac{\rho_q}{\sigma_q}\Big)\big(\zeta_l \mathrm{e}^{hD}\big) v_l &= h \sum_{m\geq 1} \frac{1}{m!} \sum_{\zeta_{l_1}\cdots\zeta_{l_m}=\zeta_l} g^{(m)}\big(y\big)\big(z_{l_1},\ldots,z_{l_m}\big) + \mathscr{O}(h^{N+1}).
\end{aligned} \tag{58}$$

Expanding the left-hand side into powers of h leads to the consideration of the series

$$\mathrm{i}\,\frac{\rho_p(\zeta_l\,\mathrm{e}^{\mathrm{i}x})}{\sigma_p(\zeta_l\,\mathrm{e}^{\mathrm{i}x})} = \lambda^p_{l0} + \lambda^p_{l1} x + \lambda^p_{l2} x^2 + \ldots, \quad \mathrm{i}\,\frac{\rho_q(\zeta_l\,\mathrm{e}^{\mathrm{i}x})}{\sigma_q(\zeta_l\,\mathrm{e}^{\mathrm{i}x})} = \lambda^q_{l0} + \lambda^q_{l1} x + \lambda^q_{l2} x^2 + \ldots$$

(note that $\lambda^p_{l0} = 0$ if $\rho_p(\zeta_l) = 0$). The symmetry of the methods implies that the coefficients λ^p_{lj} and λ^q_{lj} are real. For the conjugate root $\zeta_{-l} = \overline{\zeta_l}$ we have

$$\lambda^p_{-l,j} = (-1)^{j+1}\lambda^p_{l,j}, \qquad \lambda^q_{-l,j} = (-1)^{j+1}\lambda^q_{l,j}. \tag{59}$$

Removing in (58) the terms with $m \geq 2$, we thus obtain

$$\begin{aligned}
\ldots + \lambda^p_{l2}\,(-\mathrm{i}h)^2\,\ddot{u}_l + \lambda^p_{l1}\,(-\mathrm{i}h)\,\dot{u}_l &= \mathrm{i}h\,\big(f_p(p,q)\,u_l + f_q(p,q)\,v_l\big)\\
\ldots + \lambda^q_{l2}\,(-\mathrm{i}h)^2\,\ddot{v}_l + \lambda^q_{l1}\,(-\mathrm{i}h)\,\dot{v}_l + \lambda^q_{l0}\,v_l &= \mathrm{i}h\,\big(g_p(p,q)\,u_l + g_q(p,q)\,v_l\big)
\end{aligned} \tag{60}$$

and the same relations for l replaced by $-l$. An important ingredient for a further study is the fact that

$$\begin{aligned}
\Re\Big(\overline{z}^{\mathsf{T}} z^{(2m+1)}\Big) &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{j=0}^{2m}(-1)^j(\overline{z}^{(j)})^{\mathsf{T}} z^{(2m-j)}\Big)\\
\Im\Big(\overline{z}^{\mathsf{T}} z^{(2m)}\Big) &= \frac{1}{2\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_{j=0}^{2m-1}(-1)^j(\overline{z}^{(j)})^{\mathsf{T}} z^{(2m-j-1)}\Big)
\end{aligned} \tag{61}$$

are total differentials. We first put the main result of [9] on the long-time behavior of parasitic solution components into the context of the present investigation.

Second order Hamiltonian systems. We consider partitioned systems

$$\dot{p} = -\nabla U(q), \qquad \dot{q} = p,$$

[3] The case $\sigma_q(\zeta_l) = 0$ needs special attention, see the end of Section 3.5 or [9] for the special case of second order differential equations.

which are equivalent to second order differential equations $\ddot{q} = -\nabla U(q)$. In this case we have $g_q(p,q) = 0$ and $g_p(p,q) = I$, so that from the lower line of (60) the expression ihu_l is seen to be a linear combination of derivatives of v_l. Inserted into the upper relation of (60) this gives

$$\ldots - \lambda_{l3}\,(-\mathrm{i}h)^2\, v_l^{(3)} - \lambda_{l2}\,(-\mathrm{i}h)\,\ddot{v}_l - \lambda_{l1}\,\dot{v}_l = -\mathrm{i}h\,\nabla^2 U(q)\,v_l, \tag{62}$$

where $\lambda_{l1} = \lambda_{l1}^p \lambda_{l0}^q$, $\lambda_{l2} = \lambda_{l2}^p \lambda_{l0}^q + \lambda_{l1}^p \lambda_{l1}^q$, etc. are real coefficients. It follows from the symmetry of the Hessian matrix $\nabla^2 U(q)$ that $\Im(\bar{v}_l^{\mathsf{T}} \nabla^2 U(q)\, v_l) = 0$. Taking the scalar product of (62) with $\bar{v}_l^{\mathsf{T}}$ and considering its real part, we thus obtain

$$\ldots + h^2 \lambda_{l3}\, \Re(\bar{v}_l^{\mathsf{T}} v_l^{(3)}) - h\lambda_{l2}\, \Im(\bar{v}_l^{\mathsf{T}} \ddot{v}_l) - \lambda_{l1}\, \Re(\bar{v}_l^{\mathsf{T}} \dot{v}_l) = 0.$$

The magic formulas (61) show that the left-hand expression is a total differential. Its dominant term is the derivative of $-\lambda_{l1} \frac{1}{2} \|v_l\|^2$. The other terms are the derivative expressions containing higher derivatives of v_l. These can be eliminated with the help of the simplified modified differential equation. Because of $\lambda_{l1} \neq 0$, we thus get a formal invariant (a near invariant if the series is truncated) of the system (60), which is of the form

$$\ldots + h^2 I_{l2}(y,\mathbf{z}) + h I_{l1}(y,\mathbf{z}) + \|v_l\|^2 = I_l(y,\mathbf{z}).$$

Since all functions $I_{lj}(y,\mathbf{z})$ are bounded by a constant times $\|\mathbf{z}\|^2$ and since we obtain such a formal invariant for all components of $\mathbf{z}$, the stability assumption (SI) is proved with $C = 1 + \mathscr{O}(h)$ and for arbitrarily large M.

Remark 3. This derivation of a near invariant that is close to $\|v_l\|^2$ essentially relies on the fact that the polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ do not have common roots other than $\zeta = 1$. If, in addition to $\rho_p(\zeta_l) = 0$, also $\rho_q(\zeta_l) = 0$ would be satisfied, then the coefficient λ_{l0}^q would be zero. This would imply $\lambda_{l1} = 0$, so that the formal invariant does not contain the term $\|v_l\|^2$.

Separable Hamiltonian systems. We next consider a Hamiltonian system with

$$H(p,q) = T(p) + U(q).$$

We still consider partitioned linear multistep methods (2), where the ρ-polynomials do not have common zeros with the exeption of $\zeta = 1$. In the situation of (60) the vector v_l contains a factor h. Since $f_p(p,q) = 0$ for a separable Hamiltonian system, the differential equation for u_l contains an additional factor h. Consequently, the differential equation (54) for $\mathbf{z}$ is in fact of the form $\dot{\mathbf{z}} = hA_{h,N}^0(y)\mathbf{z}$. Therefore we have $\|\mathbf{z}(h)\| \leq \|\mathbf{z}(0)\|(1 + \mathscr{O}(h^2))$, so that the stability assumption (SI) is satisfied with $M = 1$.

Discussion of the examples of Section 1.3. In the numerical experiments of Section 1.3 we have seen situations, where the parasitic solution components remain bounded on intervals of length $\mathscr{O}(h^{-2})$. According to our Theorem 3 this requires

the stability assumption to be satisfied for $M = 2$. The system (60) is of the form

$$\begin{aligned} \lambda_{l1}^{p}\dot{u}_l &= \nabla^2 U(q)v_l + \mathscr{O}(h^2\|\mathbf{z}\|) \\ \lambda_{l0}^{q}v_l &= \mathrm{i}h\nabla^2 T(p)u_l + \mathscr{O}(h^2\|\mathbf{z}\|) \end{aligned} \tag{63}$$

which yields the differential equation

$$\dot{u}_l = \mathrm{i}\,h\,\lambda\,\nabla^2 U(q)\nabla^2 T(p)\,u_l + \mathscr{O}(h^2\|\mathbf{z}\|)$$

with $\lambda = \lambda_{l0}^{q}/\lambda_{l1}^{p}$. If the product of the two Hessian matrices is symmetric or, equivalently, if their commutator vanishes, i.e.,

$$\left[\nabla^2 U(q), \nabla^2 T(p)\right] = \nabla^2 U(q)\nabla^2 T(p) - \nabla^2 T(p)\nabla^2 U(q) = 0, \tag{64}$$

we can multiply the differential equation with $\overline{u}_l^{\mathsf{T}}$ and we obtain

$$\|u_l(h)\|^2 = \|u_l(0)\|^2 + \mathscr{O}(h^3\|\mathbf{z}(0)\|^2)$$

as a consequence of $\Im(\overline{u}_l^{\mathsf{T}}\nabla^2 U(q)\nabla^2 T(p)\,u_l) = 0$. This prove the validity of the stability assumption (SI) with $M = 2$. Unfortunately, the commutativity of the two Hessian matrices is a strong requirement and not often satisfied.

The examples (A) and (B) of Section 1.3 are separable Hamiltonian equations, which split into independent subsystems having one degree of freedom. The condition (64) is therefore trivially satisfied.

For the example (C) the condition (64) is not satisfied, so that we do not have better than $M = 1$ in the stability assumption (SI). Let us explain the behavior observed in Figure 2. The parasitic roots of method 'plmm2' are $\zeta_1 = \mathrm{i}$, $\zeta_{-1} = -\mathrm{i}$, and $\zeta_2 = -1$.

We have $\sigma_q(\zeta_2) = 0$, so that the division by $\sigma_q(\zeta_2 \mathrm{e}^{hD})$ is not permitted in (58). We thus go back to formula (42), which shows that for $\rho_q(\zeta_l) \neq 0$ and $\sigma_q(\zeta_l) = 0$ the vector v_l is an expression multiplied by h^2. Inserted into the first equation of (63) we see that the right-hand side of the differential equation for u_2 contains the factor h^2, so that $\|u_2(h)\|^2 = \|u_2(0)\|^2 + \mathscr{O}(h^3\|\mathbf{z}(0)\|^2)$.

For the root $\zeta_1 = \mathrm{i}$ we study numerically the dominant term of the parasitic solution component. We have $\lambda_{l0}^{p} = -1$ and $\lambda_{l1}^{q} = 2$ for the method 'plmm2', so that the differential equation for v_l becomes

$$\dot{v}_1 = -\frac{\mathrm{i}\,h}{2}\nabla^2 T(p)\nabla^2 U(q)\,v_1 + \mathscr{O}(h^2\|\mathbf{z}\|).$$

We neglect the $\mathscr{O}(h^2\|\mathbf{z}\|)$ term and solve the linear differential equation for v_1 numerically with the code DOPRI5 of [12]. Since the problem is chaotic, care has to be taken about the credibility of the results. We therefore solve the problem with a high accuracy requirement of $tol = 10^{-12}$ and with many different initial values of norm $\|v_1(0)\| = 1$. The result is qualitatively the same for all runs, and we plot in Figure 5 one such parasitic solution.

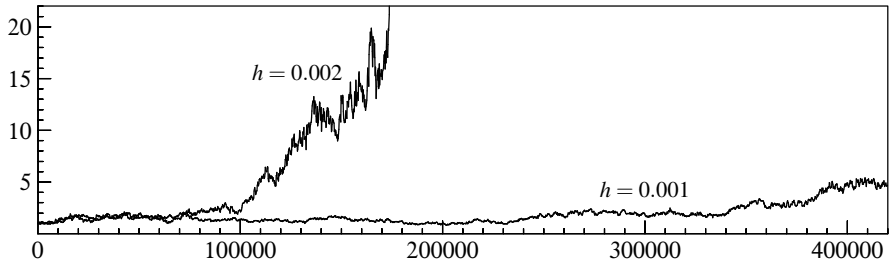


Fig. 5 Euclidean norm of the parasitic solution component v_1; data for the Hamiltonian system are as in Figure 1, problem (C); initial data for the parasitic component are normalized to $\|v_1(0)\| = 1$.

If the starting approximations for the partitioned multistep method are computed with high accuracy (what is the case for all our numerical experiments), the initial values of the parasitic solution components are of size $\mathscr{O}(h^{r+1})$ (where r denotes the order of the method). Consequently, the functions shown in Figure 5 have to be scaled with a factor $\mathscr{O}(h^{r+1})$. A comparison with Figure 2 shows that this solution, where we have removed quadratic and higher order terms in $\mathbf{z}$ as well a linear terms in $\mathbf{z}$ with a a factor of at least h^2, cannot be the reason of the exponential divergence in Figure 2. It must be a consequence of the next term having a factor h^2. This nicely explains why the parasitic solution components remain small and bounded on intervals of length $\mathscr{O}(h^{-2})$.

Conclusion

We have studied the long-time behavior of partitioned linear multistep methods applied to Hamiltonian systems. These are methods, where the momenta p and the positions q of the system are treated by two different multistep formula. It turns out that the following two properties are essential for a qualitative correct simulation over long times:

- both multistep schemes have to be symmetric;
- the generating polynomials $\rho_p(\zeta)$ and $\rho_q(\zeta)$ of the two methods are not allowed to have common zeros with the exception of $\zeta = 1$.

The study is motivated by the analysis of [9] for special multistep methods and Hamiltonian systems of the form $\ddot{q} = -\nabla U(q)$. We have extended the techniques of proof to a more general situation.

The positive insight of our investigation is that for problems having symmetries and a regular solution behavior, the numerical results concerning long-time preservation of energy and quadratic first integrals are excellent. This is remarkable, because the considered methods are explicit, of arbitrarily high order, and can be implemented very efficiently. We expect that this excellent long-time behavior

is typical for all nearly integrable systems. A more thorough investigation of this question is outside the scope of the present work.

For separable Hamiltonian systems with chaotic solution, we observed that the 'smooth' numerical solution behaves exactly like a symmetric (non-symplectic) one-step method. The parasitic solution components are typically bounded on a time interval of length $\mathcal{O}(h^{-2})$, but usually not on longer time intervals. This observation is independent of the order of the method.

Recently we have extended our numerical experiments and also the theoretical investigations to constrained Hamiltonian systems, which are differential-algebraic equations of index 3. Preliminary results are very encouraging and we expect to obtain a new efficient class of methods for such problems.

Acknowledgements We are grateful to Luca Dieci and Nicola Guglielmi, organizers of the CIME-EMS summer school on "Current challenges in stability issues for numerical differential equations", for including our research in their program. We acknowledge financial support from the Fonds National Suisse, Project No. 200020-126638 and 200021-129485.

References

1. M. J. Ablowitz and J. F. Ladik. A nonlinear difference scheme and inverse scattering. *Studies in Appl. Math.*, 55:213–229, 1976.
2. G. Akrivis, M. Crouzeix, and C. Makridakis. Implicit-explicit multistep methods for quasilinear parabolic equations. *Numer. Math.*, 82(4):521–541, 1999.
3. C. Arévalo and G. Söderlind. Convergence of multistep discretizations of DAEs. *BIT*, 35(2):143–168, 1995.
4. P. Chartier, E. Faou, and A. Murua. An algebraic approach to invariant preserving integrators: the case of quadratic and Hamiltonian invariants. *Numer. Math.*, 103:575–590, 2006.
5. G. Dahlquist. Stability and error bounds in the numerical integration of ordinary differential equations. *Trans. of the Royal Inst. of Techn., Stockholm, Sweden*, 130, 1959.
6. K. Feng. *Collected Works II*. National Defense Industry Press, Beijing, 1995.
7. E. Hairer. Backward error analysis for multistep methods. *Numer. Math.*, 84:199–232, 1999.
8. E. Hairer and C. Lubich. Long-time energy conservation of numerical methods for oscillatory differential equations. *SIAM J. Numer. Anal.*, 38:414–441, 2001.
9. E. Hairer and C. Lubich. Symmetric multistep methods over long times. *Numer. Math.*, 97:699–723, 2004.
10. E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics 31. Springer-Verlag, Berlin, 2nd edition, 2006.
11. E. Hairer, R. McLachlan, and R. Skeel. On energy conservation of the simplified Takahashi–Imada method. *M2AN Math. Model. Numer. Anal.*, 43(4):631–644, 2009.
12. E. Hairer, S. P. Nørsett, and G. Wanner. *Solving Ordinary Differential Equations I. Nonstiff Problems*. Springer Series in Computational Mathematics 8. Springer, Berlin, 2nd edition, 1993.
13. E. Hairer and C. Schober. Corrigendum to: "Symplectic integrators for the Ablowitz-Ladik discrete nonlinear Schrödinger equation" [Phys. Lett. A 259 (1999), 140–151]. *Phys. Lett. A*, 272(5-6):421–422, 2000.
14. U. Kirchgraber. Multi-step methods are essentially one-step methods. *Numer. Math.*, 48:85–90, 1986.

15. G. D. Quinlan and S. Tremaine. Symmetric multistep methods for the numerical integration of planetary orbits. *Astron. J.*, 100:1694–1700, 1990.
16. C. M. Schober. Symplectic integrators for the Ablowitz-Ladik discrete nonlinear Schrdinger equation. *Phys. Lett. A*, 259:140–151, 1999.
17. Y.-F. Tang. The symplecticity of multi-step methods. *Computers Math. Applic.*, 25:83–90, 1993.
18. D. S. Vlachos and T. E. Simos. Partitioned linear multistep method for long term integration of the *N*-body problem. *Appl. Numer. Anal. Comput. Math.*, 1(3):540–546, 2004.