Error analysis of exponential integrators for oscillatory second-order differential equations

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Abstract. In this paper we analyse a family of exponential integrators for second-order differential equations in which high-frequency oscillations in the solution are generated by a linear part. Conditions are given which guarantee that the integrators allow second-order error bounds independent of the product of the step size with the frequencies. Our convergence analysis generalises known results on the mollified impulse method by García-Archilla, Sanz-Serna and Skeel [6] and on Gautschi-type exponential integrators [12, 13].

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1. Introduction

In this paper we present an error analysis for a family of exponential integrators for the solution of systems of second-order differential equations

$$y''(t) = -Ay(t) + g(y(t)), \qquad y(t_0) = y_0, \quad y'(t_0) = y_0', \tag{1}$$

where $A = \Omega^2$ is a positive semi-definite symmetric matrix of arbitrarily large norm. Such problems have been studied in a number of papers recently, see, e.g., [1, 2, 3, 4, 6, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. So far, error bounds which do not deteriorate when the product of the step size with the frequencies of the problem become large or, in the case of resonances, close to multiples of π, have been proved for two different schemes. The first one is the *mollified impulse method* proposed and analysed by García-Archilla, Sanz-Serna and Skeel [6]. Using a different technique, Hochbruck and Lubich [13] considered a *Gautschi-type exponential integrator* and proved error bounds for a two-step formulation of the scheme. The analysis in [13] also gave new insight into the convergence of the mollified impulse method.

Recently, the implication of geometric properties like symplecticity, symmetry, or reversibility on the long-time behaviour of the schemes when applied to highly-oscillatory problems has been studied [3, 11, 12]. As a first attempt in understanding these phenomena, a model problem, which is a special case of (1),

$$y''(t) = -\begin{bmatrix} 0 & 0 \\ 0 & \omega^2 I \end{bmatrix} y(t) + g(y(t)), \qquad y(t_0) = y_0, \quad y'(t_0) = y_0', \tag{2}$$

with blocks of arbitrary dimension, was proposed. The behaviour of a whole family of exponential integrators, which includes the mollified impulse method [6] and the Gautschi-type integrator [13] as special cases, was analysed in detail for this model problem in [11]. The analysis showed that neither of the latter two methods is the best possible with respect to long-time behaviour. However, to the best of our knowledge, error bounds for the most promising methods for the general problem (1) are not known so far. Results based on the modulated Fourier expansion [3] have been proved for two-step methods for the model problem (2) only [12, Section XIII.4]. They can probably be generalised to the case that there is a *finite* number of large frequencies by using the techniques of [4].

In the present paper, we will characterise all possible methods of the family proposed in [12] which allow second-order error bounds for the general problem (1) by presenting a unified error analysis for the whole family of methods. The techniques used in [6] and [13] do not extend to this general class in an obvious way. In contrast to the analysis of [13], where the two-step version of the Gautschi-type method is considered, the present paper deals with the one-step formulation. A major advantage of our new analysis is that it does not require bounds for point-wise products of matrices and therefore, generalises to abstract differential equations, where A is an unbounded operator with infinitely many large eigenvalues directly. A conjecture posed in [13] which states that the two-step formulation of the Gautschi-type methods allows for error bounds independent of the dimension of the problem was proved by Grimm in [9].

Our paper is organised as follows: we will recall the family of methods considered here in Section 2. The main theorem and a new choice of filter function is presented in Section 3. In order to compare the performance of our scheme to known results in the literature, in particular in [12, Chapter XIII], we have chosen to show the numerical behaviour of the methods by applying it to the Fermi–Pasta–Ulam problem. The results are presented in Section 4. It turns out that, for the Fermi–Pasta–Ulam problem, our new method is the only one which is of second order *and* conserves the energy for long-time intervals. Since the proof of our main theorem is quite involved it is postponed to Section 5.

2. The integration scheme

The variation-of-constants formula

$$\begin{bmatrix} y(t) \\ y'(t) \end{bmatrix} = \begin{bmatrix} \cos(t-t_0)\Omega & \Omega^{-1}\sin(t-t_0)\Omega \\ -\Omega\sin(t-t_0)\Omega & \cos(t-t_0)\Omega \end{bmatrix} \begin{bmatrix} y(t_0) \\ y'(t_0) \end{bmatrix} + \int_{t_0}^{t} \begin{bmatrix} \Omega^{-1}\sin(t-s)\Omega \\ \cos(t-s)\Omega \end{bmatrix} g(y(s))\,ds$$

suggests the following numerical integration schemes for the solution of (1)

$$\begin{bmatrix} y_{n+1} \\ y'_{n+1} \end{bmatrix} = R(h\Omega) \begin{bmatrix} y_n \\ y'_n \end{bmatrix} + \begin{bmatrix} \frac{1}{2}h^2\Psi g(\Phi y_n) \\ \frac{1}{2}h\Big(\Psi_0 g(\Phi y_n) + \Psi_1 g(\Phi y_{n+1})\Big) \end{bmatrix}, \tag{3}$$

where

$$R(h\Omega) := \begin{bmatrix} \cos h\Omega & \Omega^{-1}\sin h\Omega \\ -\Omega\sin h\Omega & \cos h\Omega \end{bmatrix} \tag{4}$$

and

$$\Phi = \phi(h\Omega), \quad \Psi = \psi(h\Omega), \quad \Psi_0 = \psi_0(h\Omega), \quad \Psi_1 = \psi_1(h\Omega).$$

The functions ϕ, ψ, ψ_0, and ψ_1 are even analytic functions, with

$$\phi(0) = \psi(0) = \psi_0(0) = \psi_1(0) = 1,$$

bounded on the non-negative real axis. By exchanging $n \leftrightarrow n+1$ and $h \leftrightarrow -h$ in the method, it can be seen that the method is symmetric if and only if

$$\psi(\xi) = \operatorname{sinc}(\xi)\psi_1(\xi), \qquad \psi_0(\xi) = \cos(\xi)\psi_1(\xi), \tag{5}$$

where $\operatorname{sinc}\xi = \sin\xi/\xi$. A symmetric method can be cast into an equivalent two-step formulation

$$y_{n+1} - 2\cos h\Omega \cdot y_n + y_{n-1} = h^2\Psi g(\Phi y_n), \tag{6}$$

with starting values

$$y_0, \qquad y_1 = \cos h\Omega \cdot y_0 + \Omega^{-1}\sin h\Omega \cdot y'_0 + \frac{1}{2}h^2\Psi g(\Phi y_0).$$

The methods are equivalent with these initial values only. Multistep methods are usually considered to be of second order if they are of second order for arbitrary starting values that are close enough to the exact solution. According to this definition, one-step methods (3) and their two-step formulation (6) are not equivalent with respect to their non-smooth order. For example, the mollified impulse method is of second order as a one-step method, but if one uses the exact solution as starting values y_0 and y_1, the mollified impulse method is not of second order as a two-step method, cf. [13, Section 7]. Another example is the Gautschi-type exponential integrator (6) in which

$$\psi(\xi) = \operatorname{sinc}^2(\frac{1}{2}\xi), \qquad \phi(\xi) = \operatorname{sinc}(\xi)\left(1 + \frac{1}{3}\sin^2(\frac{1}{2}\xi)\right). \tag{7}$$

This method is of non-smooth second order for arbitrary starting values close enough to the exact solution. However, if we rewrite this method in the one-step form (3), then the function ψ satisfying the symmetry relation (5) yields a filter function ψ_1 that has singularities at odd integer multiples of π. This prevents the method from being of order two as a one-step method in the form (3). A different one-step formulation of the Gautschi-type method is given in [13]. Our paper focuses on one-step methods.

Symplectic methods possess a very good energy preservation for small step sizes h, whenever (1) is a Hamiltonian system. The methods are symplectic, if and only if

$$\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi), \tag{8}$$

cf. [12, p. 417]. However, with respect to oscillatory differential equations, where the product of the highest frequency in the system with the step size h is large, the situation is different. The analysis in [11] for linear problems (2), i.e. $g(y) = By$, satisfying the *finite-energy condition*

$$\frac{1}{2}\|y'(t)\|^2 + \frac{1}{2}\|\Omega y(t)\|^2 \leq \frac{1}{2}K^2, \qquad t_0 \leq t \leq t_0 + T, \tag{9}$$

shows that the numerical method conserves the total energy up to $O(h)$ for all values of $h\omega$, if and only if

$$\psi(\xi) = \operatorname{sinc}^2(\xi)\phi(\xi), \tag{10}$$

see [12, p. 449]. The relations (8) and (10) cannot be satisfied simultaneously, and symmetric methods that satisfy (10) are therefore expected to possess favourable energy-conservation properties. It is not clear to us whether condition (10) is sufficient to guarantee energy preservation for general systems (1). But the analysis in [11] clearly shows that these methods are at least preferable to symplectic methods for oscillatory differential equations.

3. Finite-time error analysis

The result stated in this section makes no smoothness assumptions about the highly-oscillatory solution y except (9). The even analytic functions defining the integrator (3) are assumed to be bounded on the non-negative real axis, i.e. $\chi = \phi,\ \psi, \psi_0,\ \psi_1$ satisfy

$$\max_{\xi \geq 0} |\chi(\xi)| \leq M_1, \tag{11}$$

for some constant M_1. Moreover, we assume $\phi(0) = 1$, thus the existence of a constant M_2 such that

$$\max_{\xi \geq 0} \left| \frac{\phi(\xi) - 1}{\xi} \right| \leq M_2. \tag{12}$$

In addition, we assume

$$\max_{\xi \geq 0} \left| \frac{1}{\sin \frac{\xi}{2}} \left(\operatorname{sinc}^2 \frac{\xi}{2} - \psi(\xi) \right) \right| \leq M_3 \tag{13}$$

and

$$\max_{\xi \geq 0} \left| \frac{1}{\xi \sin \frac{\xi}{2}} \left(\operatorname{sinc} \xi - \chi(\xi) \right) \right| \leq M_4, \qquad \chi = \phi,\ \psi_0,\ \psi_1. \tag{14}$$

The assumptions made so far are necessary to prove second-order error bounds for the positions $y_n \approx y(t_n)$. In order to verify first order error bounds for the velocities, we assume

$$\max_{\xi \geq 0} |\xi\, \psi(\xi)| \leq M_5, \qquad \max_{\xi \geq 0} \left| \frac{\xi}{\sin \frac{\xi}{2}} \left(\operatorname{sinc}^2 \frac{\xi}{2} - \psi(\xi) \right) \right| \leq M_6, \tag{15}$$

and

$$\max_{\xi \geq 0} \left| \frac{1}{\sin \frac{\xi}{2}} \left(\operatorname{sinc} \xi - \psi_i(\xi) \right) \right| \leq M_7, \qquad i = 0, 1. \tag{16}$$

(16) is a consequence of (14), but possibly with $M_7 > M_4$. The constants M_1 to M_7 only depend on the choice of the analytic functions. It is easy to find analytic functions such that

$$M := \max_{i=1,\dots,7} M_i$$

is a small constant; examples will be given in Section 4.

Theorem 1. *In* (1)*, let $A = \Omega^2$ be an arbitrary symmetric positive semi-definite matrix. Suppose g, g_y and g_{yy} are bounded in the Euclidean norm or the norms induced by the Euclidean norm, respectively. Assume the solution y satisfies the finite-energy condition* (9)*. If the even analytic functions of scheme* (3) *satisfy* (11), (12), (13), *and* (14), *then*

$$\|y(t_n) - y_n\| \leq h^2\, C, \qquad t_0 \leq t_n = t_0 + nh \leq t_0 + T.$$

The constant C only depends on $T, K, M_1, \dots, M_4$, $\|g\|, \|g_y\|$, and $\|g_{yy}\|$. If, in addition, (15) *and* (16) *are satisfied, then*

$$\|y'(t_n) - y'_n\| \leq h\, \widetilde{C}, \qquad t_0 \leq t_n = t_0 + nh \leq t_0 + T.$$

The constant $\widetilde{C}$ only depends on T, K, M, $\|g\|$, $\|g_y\|$, and $\|g_{yy}\|$.

The proof of this theorem will be given in Section 5 below.

It is important to note that the constants $C, \widetilde{C}$ only depend on the finite energy of the exact solution, the choice of the filter functions, and the smoothness of the nonlinearity g but not on the norm of A or on higher derivatives of the exact solution. This property is very desirable. For example, if system (1) is a semi-discretisation of a wave equation, then the bounds are independent of the mesh size used for the spatial discretisation.

If the method is symmetric (5) and symplectic (8), with $\phi(\xi)$ vanishing at integer multiples of π, then (11)–(16) are satisfied. These are the assumptions stated in [6] and thus the results therein are a special case of our general Theorem 1.

However, it was shown in [11], that symmetric and symplectic methods cannot preserve the energy for linear systems (1) with $g(y) = By$ for large step sizes. Interestingly, a symmetric method which additionally satisfies (10) instead of the symplecticity condition (8), with $\phi(\xi)$ vanishing at integer multiples of π, fulfils (11)–(16). Therefore, the method with

$$\phi(\xi) = \operatorname{sinc}\xi, \qquad \psi(\xi) = \operatorname{sinc}^2\xi\,\phi(\xi), \tag{17}$$

where ψ_0 and ψ_1 chosen such that the method is symmetric (5), fulfils all conditions of Theorem 1 and thus allows second-order error bounds independent of the frequencies. Moreover, it satisfies (10), so that long-time energy preservation similar to the method proposed in [11] can be expected. The latter method does not allow a second-order error bound independent of the norm of Ω. This can be seen in Figure 2 in the plot labelled (E), where the resonances appear exactly at the points where condition (14) for $\phi(\xi) = 1$ fails to hold. A numerical comparison of the new method with existing schemes is given in the following section.

4. Numerical Experiment

We consider the Fermi–Pasta–Ulam problem, since this allows comparisons to earlier work, in particular in [12]. We refer the reader to [12] for a detailed description of this problem. To avoid confusion with the notation therein, we denote our new method with (G). Since we only consider symmetric methods, it is enough to give the analytic functions ψ and ϕ to determine the one-step method uniquely:

(A)	$\psi(\xi) = \operatorname{sinc}^2(\frac{1}{2}\xi)$	$\phi(\xi) = 1$	Gautschi [7]
(B)	$\psi(\xi) = \operatorname{sinc}(\xi)$	$\phi(\xi) = 1$	Deuflhard [5]
(C)	$\psi(\xi) = \operatorname{sinc}(\xi)\phi(\xi)$	$\phi(\xi) = \operatorname{sinc}(\xi)$	García-Archilla et al. [6]
(D)	$\psi(\xi) = \operatorname{sinc}^2(\frac{1}{2}\xi)$	$\phi(\xi)$of (7)	Hochbruck, Lubich [13]
(E)	$\psi(\xi) = \operatorname{sinc}^2(\xi)$	$\phi(\xi) = 1$	Hairer, Lubich [11]
(G)	$\psi(\xi) = \operatorname{sinc}^3(\xi)$	$\phi(\xi) = \operatorname{sinc}(\xi)$	

Figure 1 shows the maximum error of the total energy as a function of the scaled frequency $h\omega$ on the interval $[0, 1000]$. Only methods (E) and (G) show a uniformly good energy preservation for all frequencies. To compare the accuracy, we used the Fermi–Pasta–Ulam problem with very stiff springs, $\omega = 1000$. Methods $(C), (D)$, and (G) are the only methods with uniformly good accuracy for all frequencies, as can be seen in Figure 2. Method (G) is the only method that has a good behaviour with respect to accuracy and energy conservation uniformly in the frequencies for the Fermi–Pasta–Ulam problem. Theorem 1 and the result about the conservation of energy for linear problems in [11] suggested this new method. The Fermi–Pasta–Ulam problem has another nearly conserved quantity, the oscillatory energy

$$I = I_1 + I_2 + I_3 \quad \text{with} \quad I_j = \frac{1}{2}(y')^2_{2,j} + \frac{1}{2}\omega^2 y^2_{2,j}.$$

Figure 3 shows the maximum error of the oscillatory energy. It can be seen that method (G) is the only method that has a uniformly good preservation of the oscillatory energy for $h\omega$ bounded away from zero. This good performance compared to the other methods comes as a surprise. In [11], Hairer and Lubich could show that no method can uniformly conserve the oscillatory energy in an interval of length more than 2π for linear systems. Methods (A)-(F) of [11] show severe resonances for the oscillatory energy in any interval of length more than 2π in the nonlinear Fermi–Pasta–Ulam problem. The new method (G) does not show severe resonances in the oscillatory energy for the Fermi–Pasta–Ulam Problem even on a finer temporal grid than that shown in the figure.

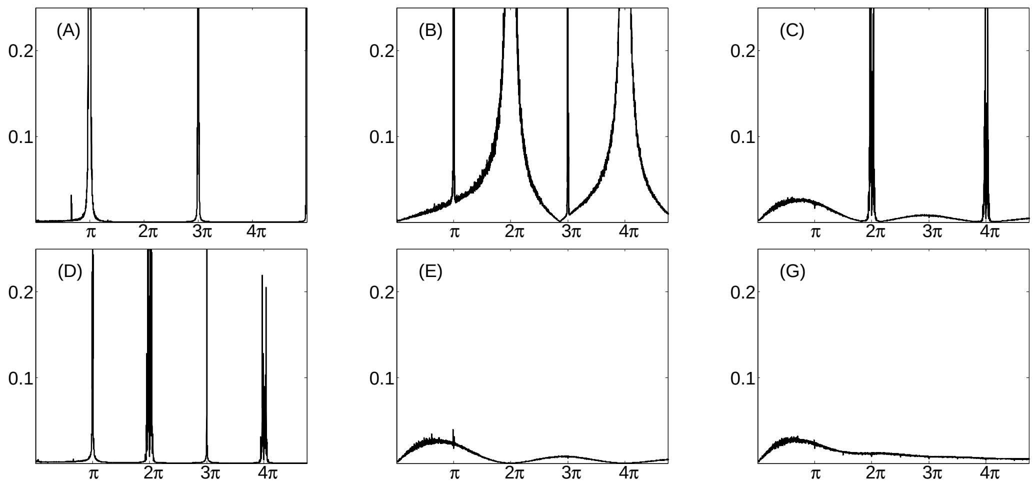

Figure 1. Maximum error of total energy on the interval $[0, 1000]$ as a function of $h\omega$ (step size $h = 0.02$).

5. Proof of Theorem 1

The proof of Theorem 1 is tedious and split into several lemmas. In the following, C is a generic constant, depending only on the constants mentioned in Theorem 1, that takes on different values on different occurrences. By assumption, $\Omega = A^{1/2}$ is symmetric, positive semi-definite. If Ω is singular, $\Omega^{-1}\sin t\Omega$ is interpreted as $t \operatorname{sinc} t\Omega$, which is defined for an arbitrary matrix Ω.

Proof of Theorem 1. Substitution of the exact solution into the integration scheme (3) with $R = R(h\Omega)$ gives

$$\begin{bmatrix} y(t_{n+1}) \\ y'(t_{n+1}) \end{bmatrix} = R \begin{bmatrix} y(t_n) \\ y'(t_n) \end{bmatrix} + \begin{bmatrix} \frac{1}{2}h^2\Psi g(\Phi y(t_n)) \\ \frac{1}{2}h\Big(\Psi_0 g(\Phi y(t_n)) + \Psi_1 g(\Phi y(t_{n+1}))\Big) \end{bmatrix} + \begin{bmatrix} d_n \\ d'_n \end{bmatrix},$$

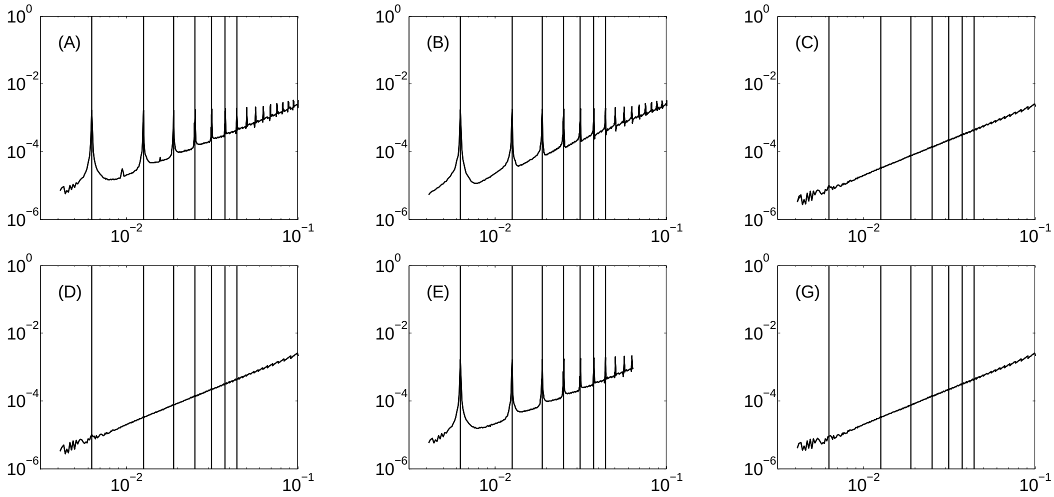

Figure 2. Global error in positions at $t = 1$ of the methods versus step size

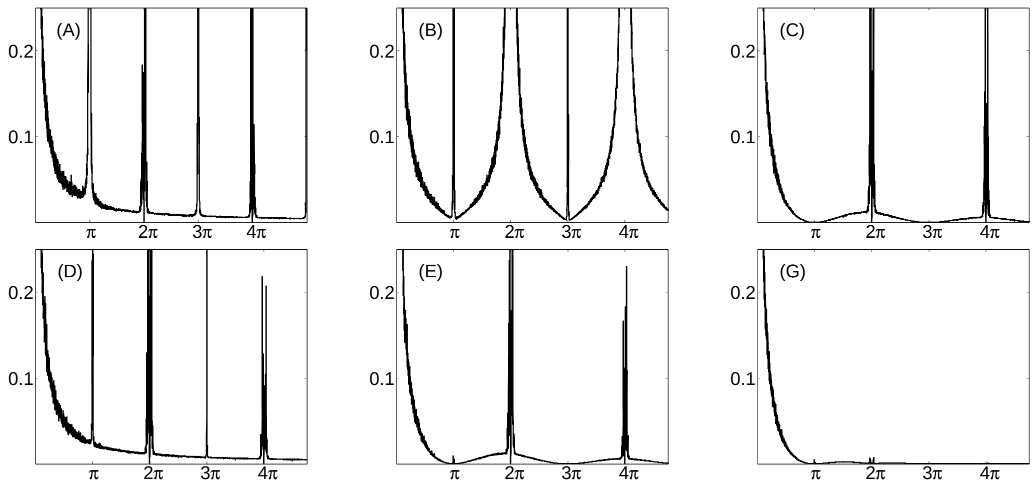

Figure 3. Maximum deviation of the oscillatory energy on the interval $[0, 1000]$ as a function of $h\omega$ (step size $h = 0.02$).

with the defects d_n and d_n'. Subtraction of equation (3) and summation leads to

$$\begin{bmatrix} e_{n+1} \\ e_{n+1}' \end{bmatrix} = R^{n+1} \begin{bmatrix} e_0 \\ e_0' \end{bmatrix} + \sum_{j=0}^{n} R^{n-j} \begin{bmatrix} \frac{1}{2}h^2 \Psi F_j e_j \\ \frac{1}{2}h\Psi_0 F_j e_j + \frac{1}{2}h\Psi_1 F_{j+1} e_{j+1} \end{bmatrix} + \begin{bmatrix} D_n \\ D_n' \end{bmatrix}, \quad (18)$$

where $e_n := y(t_n) - y_n$ and $e_n' := y'(t_n) - y_n'$,

$$F_n := \int_0^1 g_y\Big(\Phi(y_n + ue_n)\Big)\, du \cdot \Phi, \qquad \|F_n\| \le \|g_y\| M_1,$$

and

$$\begin{bmatrix} D_n \\ D_n' \end{bmatrix} = \sum_{j=0}^{n} \begin{bmatrix} \cos(n-j)h\Omega & \Omega^{-1}\sin(n-j)h\Omega \\ -\Omega\sin(n-j)h\Omega & \cos(n-j)h\Omega \end{bmatrix} \begin{bmatrix} d_j \\ d_j' \end{bmatrix}. \quad (19)$$

The proof proceeds as follows: we start by giving expressions for d_j and d'_j in Lemma 1 and Lemma 2, respectively. Using these expressions, we provide bounds for the four sums in the right-hand side of (19) in Lemmas 3–6. These bounds yield

$$\|D_n\| \le Ch^2 \qquad \text{and} \qquad \|D'_n\| \le Ch.$$

Due to $e_0 = e'_0 = 0$ the recursion (18) reads

$$e_{n+1} = h\sum_{j=1}^{n} L_j e_j + D_n,$$

where

$$L_j := \frac{1}{2}(h\cos(n-j)h\Omega \cdot \Psi + (n-j)h\,\mathrm{sinc}(n-j)h\Omega \cdot \Psi_0 \\ + (n+1-j)h\,\mathrm{sinc}(n+1-j)h\Omega \cdot \Psi_1))F_j.$$

This yields

$$\|L_j\| \le \frac{3}{2}T\|g_y\|M_1^2,$$

so that $\|e_n\| \le Ch^2$ follows from Gronwall's Lemma. Assumption (15) and the recursion for e'_n finally shows $\|e'_n\| \le Ch$. □

Lemma 1. *The defects d_n can be written as*

$$d_n = \frac{1}{2}h^2\left(\mathrm{sinc}^2\frac{h}{2}\Omega - \Psi\right)g(\Phi y(t_n)) + h^3 z_n,$$

with

$$\|z_n\| \le C \qquad \textit{and} \qquad \|h\Omega z_n\| \le C.$$

Thereby C only depends on K, $\|g_y\|$, and M_2.

Proof. With the help of the variation-of-constants formula, the defects d_n are given as

$$d_n = \int_{t_n}^{t_{n+1}} \Omega^{-1}\sin\left((t_{n+1}-s)\Omega\right)\, g(y(s))\,ds - \frac{1}{2}h^2\Psi g(\Phi y(t_n)).$$

Transforming the integration interval to $[0,1]$, applying the variation-of-constants formula and Taylor expansion for g leads to the representation given above with

$$z_n = \int_0^1 (1-s)\mathrm{sinc}\,h(1-s)\Omega \cdot \Bigg(\\ \int_0^1 g_y(y(t_n) + u(y(t_n+hs) - y(t_n)))\,du\Big[s\int_0^1 y'(t_n+hsv)\,dv\Big] \\ - \int_0^1 g_y(y(t_n) + u(\Phi - I)y(t_n))\,du\Big[\frac{\Phi - I}{h\Omega}\,\Omega y(t_n)\Big]\Bigg)\,ds.$$

Hence we have

$$\|z_n\| \le \frac{1}{2}\left(\frac{1}{3} + M_2\right)\|g_y\|\,K.$$

The bound for $\|h\Omega z_n\|$ follows by multiplying the equation above with $h\Omega$ since $(1-s)$ drops out and sinc turns into sin. □

Lemma 2. *The defects d'_n can be written as*

$$
\begin{aligned}
d'_n = {} & \frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_0\Big) g(\Phi y(t_n)) + \frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_1\Big) g(\Phi y(t_n+h)) \\
& + \frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot g_y(\Phi y(t_n)) \; \cdot \\
& \qquad \Big[\Big(\cos hs\Omega - \Phi\Big)y(t_n) + \Omega^{-1}\sin hs\Omega \cdot y'(t_n)\Big]\, ds \\
& + \frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot g_y(\Phi y(t_{n+1})) \; \cdot \\
& \qquad \Big[\Big(\cos h(s-1)\Omega - \Phi\Big)y(t_n+h) \\
& \qquad\qquad + \Omega^{-1}\sin h(s-1)\Omega \cdot y'(t_n+h)\Big]\, ds + h^3 z'_n,
\end{aligned}
$$

with $\|z'_n\| \le C$. Here C only depends on K, $\|g\|$, $\|g_y\|$, $\|g_{yy}\|$, and M_2.

Proof. The defects are given as

$$
\begin{aligned}
d'_n = {} & \int_0^h \cos(h-s)\Omega \cdot g(y(t_n+s))\, ds - \frac{1}{2}h\Big(\Psi_0 g(\Phi y(t_n)) + \Psi_1 g(\Phi y(t_{n+1}))\Big) \\
= {} & \frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_0\Big) g(\Phi y(t_n)) + \frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_1\Big) g(\Phi y(t_n+h)) \\
& + \frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot (g(y(t_n+hs)) - g(\Phi y(t_n)))\, ds \\
& + \frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot (g(y(t_n+hs)) - g(\Phi y(t_n+h)))\, ds.
\end{aligned}
$$

Taylor expansion for g and the variation-of-constants formula lead to the representation given above with $\|z'_n\| \le \frac{1}{6}\|g\|\|g_y\| + \|g_{yy}\|\,(1+M_2)^2\, K^2$. □

Lemma 3. *For n with $0 \le (n+1)h \le T$, it holds that*

$$
\left\| \sum_{j=0}^{n} \cos(n-j)h\Omega \cdot d_j \right\| \le Ch^2,
$$

where C depends on K, T, $\|g\|$, $\|g_y\|$, M_1, M_2, and M_3.

Proof. According to Lemma 1, we have

$$
\left\| h^3 \sum_{j=0}^{n} \cos(jh\Omega) \cdot z_{n-j} \right\| \le TCh^2,
$$

where C depends on K,$\|g_y\|$ and M_2. Thus it remains to bound

$$
\frac{1}{2}h^2 \sum_{j=0}^{n} \cos(jh\Omega) \left(\operatorname{sinc}^2 \frac{h}{2}\Omega - \Psi\right) g_{n-j} =: \frac{1}{2}h^2 u_n, \qquad g_j = g(\Phi y(t_j)).
$$

By partial summation, u_n can be written as

$$u_n = E_n(h\Omega)g_0 + \sum_{j=0}^{n-1} E_j(h\Omega)(g_{n-j} - g_{n-j-1}),$$

where

$$E_j(\xi) := \frac{1}{2\sin(\frac{\xi}{2})}\left(\mathrm{sinc}^2\frac{\xi}{2} - \psi(\xi)\right)\left(\sin(j\xi + \frac{\xi}{2}) + \sin\frac{\xi}{2}\right).$$

Due to (13), we have $\|E_j(h\Omega)\| \le M_3$ and therefore

$$\|u_n\| \le M_3\|g\| + \sum_{j=0}^{n-1} M_3 M_1 \|g_y\| hK \le M_3(\|g\| + TM_1\|g_y\|K).$$

This completes the proof. □

Lemma 4. *For n with $0 \le (n+1)h \le T$, it holds that*

$$\left\| \sum_{j=0}^{n} \Omega^{-1}\sin(n-j)h\Omega \cdot d_j' \right\| \le Ch^2,$$

where C depends on T, K, $\|g\|$, $\|g_y\|$, $\|g_{yy}\|$, M_1, M_2, and M_4.

Proof. According to Lemma 2, it remains to bound

$$\sum_{j=0}^{n}\Omega^{-1}\sin(n-j)h\Omega \cdot \left\{\frac{1}{2}h\Big(\mathrm{sinc}\, h\Omega - \Psi_0\Big)g(\Phi y(t_j))\right. \tag{20}$$

$$+\frac{1}{2}h\Big(\mathrm{sinc}\, h\Omega - \Psi_1\Big)g(\Phi y(t_j + h)) \tag{21}$$

$$+\frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot g_y(\Phi y(t_j)) \cdot \tag{22}$$

$$\Big[\Big(\cos hs\Omega - \Phi\Big)y(t_j) + \Omega^{-1}\sin hs\Omega \cdot y'(t_j)\Big]\, ds$$

$$+\frac{1}{2}h\int_0^1 \cos h(1-s)\Omega \cdot g_y(\Phi y(t_{j+1})) \cdot$$

$$\Big[\Big(\cos h(s-1)\Omega - \Phi\Big)y(t_j + h) \tag{23}$$

$$\left. + \Omega^{-1}\sin h(s-1)\Omega \cdot y'(t_j + h)\Big]\, ds\right\}.$$

The first and the second sum within the curly braces, (20) and (21), can be seen to be bounded by partial summation as in the lemma above. The third and the fourth term, (22) and (23), require more work. The third term (22) can be written as

$$a_n = a_n^{(1)} + a_n^{(2)},$$

where $G_j = g_y(\Phi y(t_j))$ and

$$a_n^{(1)} = \frac{1}{2}h^3\sum_{j=0}^{n}\sin(n-j)h\Omega \cdot \int_0^1 (1-s)\left(\frac{\cos h(1-s)\Omega - I}{h(1-s)\Omega}\right)G_j \cdot$$

$$\left[s\frac{\cos hs\Omega - I}{hs\Omega}\Omega y(t_j) + \frac{I - \phi(h\Omega)}{h\Omega}\Omega y(t_j) + s\,\mathrm{sinc}\, hs\Omega \cdot y'(t_j)\right] ds,$$

and

$$a_n^{(2)} = \frac{1}{2}h\sum_{j=0}^{n}\Omega^{-1}\sin(n-j)h\Omega\cdot\int_0^1 G_j\left[(\cos hs\Omega-\Phi)y(t_j)+\Omega^{-1}\sin hs\Omega\cdot y'(t_j)\right]ds.$$

Here, we wrote $1/\Omega$ instead of Ω^{-1} in order to improve the readability. We have

$$\|a_n^{(1)}\| \le \frac{1}{2}h^2T\left(\frac{1}{3}+M_2\right)\|g_y\|K.$$

Analogously, the fourth term, (23), can be written as

$$b_n = b_n^{(1)} + b_n^{(2)},$$

where

$$\begin{aligned} b_n^{(1)} = \; & \frac{1}{2}h^3\sum_{j=0}^{n}\sin(n-j)h\Omega\cdot\int_0^1(1-s)\left(\frac{\cos h(1-s)\Omega-I}{h(1-s)\Omega}\right)G_{j+1}\cdot \\ & \Big[(s-1)\frac{\cos h(s-1)\Omega-I}{h(s-1)\Omega}\Omega y(t_{j+1})+\frac{I-\phi(h\Omega)}{h\Omega}\Omega y(t_{j+1}) \\ & +(1-s)\operatorname{sinc} hs\Omega\cdot y'(t_{j+1})\Big]\,ds \end{aligned}$$

and

$$\begin{aligned} b_n^{(2)} = \; & \tfrac{1}{2}h\sum_{j=0}^{n}\Omega^{-1}\sin(n-j)h\Omega\cdot \\ & \int_0^1 G_{j+1}\left[(\cos h(s-1)\Omega-\Phi)y(t_{j+1})+\Omega^{-1}\sin h(s-1)\Omega\cdot y'(t_{j+1})\right]ds. \end{aligned}$$

One readily observes

$$\|b_n^{(1)}\| \le \frac{1}{2}h^2T\left(\frac{2}{3}+M_2\right)\|g_y\|K.$$

Hence it remains to bound $a_n^{(2)}+b_n^{(2)}$. Using

$$\int_0^1\cos hs\Omega\,ds = \int_0^1\cos h(s-1)\Omega\,ds = \operatorname{sinc} h\Omega$$

and

$$\int_0^1\Omega^{-1}\sin hs\Omega\,ds = -\int_0^1\Omega^{-1}\sin h(s-1)\Omega\,ds = \frac{h}{2}\operatorname{sinc}^2\frac{h}{2}\Omega,$$

one can rewrite

$$\begin{aligned} a_n^{(2)}+b_n^{(2)} = \; & \frac{1}{2}h\sum_{j=0}^{n}W_{n-j}\,G_j\,(\operatorname{sinc} h\Omega-\Phi)\,y(t_j) && (24)\\ & +\frac{1}{2}h\sum_{j=0}^{n}W_{n-j}\,G_{j+1}\,(\operatorname{sinc} h\Omega-\Phi)\,y(t_{j+1}) && (25)\\ & +\frac{h^2}{4}\sum_{j=0}^{n}W_{n-j}\,G_j\operatorname{sinc}^2\frac{h}{2}\Omega\cdot y'(t_j) && (26)\\ & -\frac{h^2}{4}\sum_{j=0}^{n}W_{n-j}\,G_{j+1}\operatorname{sinc}^2\frac{h}{2}\Omega\cdot y'(t_{j+1}), && (27) \end{aligned}$$

where

$$W_j := \Omega^{-1} \sin jh\Omega.$$

Since (26)–(27) can be written as

$$\frac{h^2}{4} W_n \, G_0 \operatorname{sinc}^2 \frac{h}{2}\Omega \cdot y'(t_0) + \frac{h^2}{4} \sum_{j=1}^{n} (W_{n-j} - W_{n+1-j}) \; G_j \operatorname{sinc}^2 \frac{h}{2}\Omega \cdot y'(t_j)$$

and

$$\|W_{n-j} - W_{n+1-j}\| = \left\| h \int_0^1 \cos h(n-j+s)\Omega \, ds \right\| \le h \quad \text{and} \quad \|W_j\| \le T,$$

the sums in (26) and (27) are bounded. After once more applying the variation-of-constants formula to $y(t_j)$ in (24) and using a trigonometric identity, one has to bound

$$\begin{aligned} &\frac{h^2}{2} \sum_{j=0}^{n} W_{n-j} \, G_j \; (\operatorname{sinc} h\Omega - \Phi) \, \frac{1}{h\Omega} \cos(t_j - t_0)\Omega \, w_j^1 \\ +&\frac{h^2}{2} \sum_{j=0}^{n} W_{n-j} \, G_j \; (\operatorname{sinc} h\Omega - \Phi) \, \frac{1}{h\Omega} \sin(t_j - t_0)\Omega \, w_j^2, \end{aligned}$$

where

$$\begin{aligned} w_j^1 &:= \Omega y(t_0) + \int_{t_0}^{t_j} \sin(t_0 - s)\Omega \cdot g(y(s)) \, ds, \\ w_j^2 &:= y'(t_0) + \int_{t_0}^{t_j} \cos(t_0 - s)\Omega \cdot g(y(s)) \, ds. \end{aligned}$$

Since

$$\|W_{j+1} - W_j\| \le hC \qquad \text{and} \qquad \|w_{j+1}^{1,2} - w_j^{1,2}\| \le hC,$$

partial summation with the sums

$$\sum_{j=0}^{n} (\operatorname{sinc} \xi - \phi(\xi)) \, \frac{1}{\xi} \cos j\xi \quad \text{and} \quad \sum_{j=0}^{n} (\operatorname{sinc} \xi - \phi(\xi)) \, \frac{1}{\xi} \sin j\xi,$$

(due to (14)), shows the bound. (25) is bounded analogously. □

Lemma 5. *For n with $0 \le (n+1)h \le T$, it holds that*

$$\left\| \sum_{j=0}^{n} \Omega \sin(n-j)h\Omega \cdot d_j \right\| \le Ch,$$

where C depends on T, K, $\|g\|$, $\|g_y\|$, M_1, M_2, and M_6.

Proof. According to Lemma 1,

$$\left\| h^2 \sum_{j=0}^{n} \sin jh\Omega \cdot (h\Omega z_{n-j}) \right\| \le hTC,$$

where C depends on K, $\|g_y\|$, and M_2, we have to bound

$$\frac{1}{2} h \sum_{j=0}^{n} (h\Omega) \sin jh\Omega \cdot \left(\operatorname{sinc}^2 \frac{h}{2}\Omega - \Psi \right) \, g_{n-j} =: \frac{1}{2} h v_n.$$

By partial summation, v_n can be written as

$$v_n = E'_n(h\Omega)g_0 + \sum_{j=0}^{n-1} E'_j(h\Omega)(g_{n-j} - g_{n-j-1}),$$

where

$$E'_j(\xi) := \frac{-\xi}{2\sin(\frac{\xi}{2})} \left(\operatorname{sinc}^2\frac{\xi}{2} - \psi(\xi)\right)\left(\cos(j\xi + \frac{\xi}{2}) - \cos\frac{\xi}{2}\right).$$

Due to (15), we have $\|E'_j(h\Omega)\| \le M_6$ and therefore

$$\|v_n\| \le M_6\|g\| + \sum_{j=0}^{n-1} M_6 M_1 \|g_y\| hK \le M_6(\|g\| + TM_1\|g_y\|K)$$

yields the desired result. □

Lemma 6. *For n with $0 \le (n+1)h \le T$, it holds that*

$$\left\|\sum_{j=0}^{n} \cos(n-j)h\Omega \cdot d'_j\right\| \le Ch,$$

where C depends on T, K, $\|g\|$, $\|g_y\|$, $\|g_{yy}\|$, M_1, M_2, and M_7.

Proof. From Lemma 2 we have

$$\sum_{j=0}^{n} \cos(n-j)h\Omega \cdot \left\{\frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_0\Big)g(\Phi y(t_j)) \right.$$
$$\left. + \frac{1}{2}h\Big(\operatorname{sinc} h\Omega - \Psi_1\Big)g(\Phi y(t_j + h))\right\}.$$

This can be bounded by using partial summation. □

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