ESAIM: M2AN 53 (2019) 197–218
https://doi.org/10.1051/m2an/2018050

ESAIM: Mathematical Modelling and Numerical Analysis
www.esaim-m2an.org

A POSTERIORI ERROR ESTIMATION FOR MAGNUS-TYPE INTEGRATORS

Winfried Auzinger[1], Harald Hofstätter[2], Othmar Koch[2,*], Michael Quell[1] and Mechthild Thalhammer[3]

Abstract. We study high-order Magnus-type exponential integrators for large systems of ordinary differential equations defined by a time-dependent skew-Hermitian matrix. We construct and analyze defect-based local error estimators as the basis for adaptive stepsize selection. The resulting procedures provide *a posteriori* information on the local error and hence enable the accurate, efficient, and reliable time integration of the model equations. The theoretical results are illustrated on two numerical examples.

Mathematics Subject Classification. 65L05, 65L20, 65L50, 65L70.

Received December 20, 2017. Accepted August 25, 2018.

1. Introduction and overview

Problem. We study systems of linear ordinary differential equations

$$\begin{cases} \psi'(t) = A(t)\,\psi(t) = -\,\mathrm{i}\,H(t)\,\psi(t), \qquad t > t_0, \\ \psi(t_0) = \psi_0 \ \text{ given}, \end{cases} \tag{1.1}$$

defined by a time-dependent Hermitian matrix $H\colon \mathbb{R} \to \mathbb{C}^{d\times d}$. Although the considerations below also apply to the situation of general $A(t)$, the assumption of a Schrödinger type model avoids the difficulty of having to take into account possible order reduction [28] and guarantees a unitary evolution. It is moreover strongly motivated by the applications in solid state physics in our interest, which involve Hubbard models of electrons in a solid.

The evolution operator (*i.e.*, the fundamental solution) $\mathcal{E} = \mathcal{E}(\tau; t_0)$ of the system (1.1) is characterized by the relation

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\mathcal{E}(\tau; t_0) = A(t_0+\tau)\,\mathcal{E}(\tau; t_0), \qquad \mathcal{E}(0, t_0) = \mathrm{Id}, \tag{1.2}$$

with "relative" time τ and "absolute" time $t = t_0 + \tau$, such that the solution of the initial value problem (1.1) is given by

$$\psi(t) = \psi(t_0+\tau) = \mathcal{E}(\tau; t_0)\,\psi_0.$$

Keywords and phrases. Non-autonomous linear differential equations, magnus-type integrators, *a posteriori* local error estimation, asymptotical correctness, adaptive stepsize selection.

[1] Technische Universität Wien, Institut für Analysis und Scientific Computing, Wiedner Hauptstraße 8-10, 1040 Wien, Austria.

[2] Universität Wien, Fakultät für Mathematik, Oskar-Morgenstern-Platz 1, 1090 Wien, Austria.

[3] Leopold-Franzens Universität Innsbruck, Institut für Mathematik, Technikerstraße 13, 6020 Innsbruck, Austria.

*Corresponding author: `othmar@othmar-koch.org`

For $A(t)$ of the form (1.1), the evolution operator $\mathcal{E}(\tau; t_0)$ is unitary.

Magnus-type integrators. The numerical solution of large linear systems of the type (1.1) has been extensively studied in the literature. Attention has recently focussed on *commutator-free Magnus-type methods* (CFM) introduced in [13]. These are constructed as compositions of exponentials of linear combinations of $A(t)$ evaluated at different times t. Earlier mathematical work has centered around the construction of CFM methods which are convenient to evaluate without storing excessive intermediate results, where the optimal balance between computational effort and accuracy is sought. Already in [13], the coefficients for high-order CFM methods were derived based on nonlinear optimization of the free parameters in the order conditions to minimize local error constants. With this objective, methods of orders 4–8 were constructed in [1], and applied to strongly correlated electron systems in [2].

Alternative approaches to the construction of favorable integrators based on the evaluation of exponentials rely on the Magnus expansion. In [10] the algebraic framework underlying a systematic construction of classical Magnus integrators is discussed. The seminal references to the classical Magnus approach are [23, 27], where the former in particular reveals the underlying algebraic structure. In [12], unconventional schemes involving evaluation of some commutators are introduced which are favorable for matrices of a certain structure (where commutators contribute additional powers in the stepsize). Generally, it is difficult to assess the tradeoff between the incorporation of commutators, which are usually expensive to compute and store, and the use of additional exponentials in commutator-free methods, see for example [12,15]. A similar problem-dependent tradeoff between evaluation of commutators and computation of exponentials also has to be taken into account in the construction of error estimators, see Section 3 below.

Yet another interesting approach was applied to the Schrödinger equation in [6, 7], where all the calculations are performed in the underlying Lie algebra, and practical evaluation of the arising integrals is deferred to the last stage, see also [22]. This leads to the derivation of particular Magnus-type integrators in [7].

An *a priori* theoretical error analysis for classical Magnus integrators of second and fourth order has first been given in [20] for discretizations of Schrödinger equations. The critical quantities appearing in the error bounds involve commutators such as $[A(t), A(t')]$ of the system matrix evaluated at different time points, which are estimated under appropriate regularity assumptions on the exact solution. The proof is based on estimates of the truncation error of the (infinite) Magnus series and estimates of the quadrature error in an integral representation of the remainder. The mathematical error analysis implies a mild stepsize restriction for methods of higher order. The analysis has been extended to parabolic problems in [28], where order reductions are observed, however. In this paper, we construct and analyze defect-based error estimators within a general framework that makes it possible to cover both classical and commutator-free Magnus-type integrators. Although we do not explicitly elaborate on non-standard integrators as introduced in [12], our approach for the construction of error estimators extends also to such classes of methods.

Error estimation. Reliable error estimation to serve as the basis for adaptive step-size selection for the time propagation is of particular value in large-scale applications. Previous work, however, is mainly concerned with the derivation of *a priori* error bounds, but does not treat the construction of *a posteriori* error estimators which were successfully applied for instance for exponential operator splitting methods [4, 5]. *A posteriori* error estimation and adaptive step selection for Magnus-type integrators is for instance discussed in [25], where classical Magnus integrators are endowed with a global error estimator based on integration of an adjoint problem as suggested in [14]. In [11], an economical error estimator is proposed which is also particular to classical Magnus integrators, and does not extend to the case based on more than one exponential. We will only briefly touch the question of the implied trade-off in the efficiency as compared to our proposed estimators in Section 3.4, more so since our main focus is on commutator-free integrators.

Alternatively to the Magnus-type approaches, splitting methods could be used to eliminate the time-dependence by freezing the independent variable and propagating it separately, see [9]. This allows to employ efficient high-order adaptive splitting methods proposed and analyzed for instance in [3, 5]. For these, a large body of theory has been developed in recent years, see for instance [8, 16, 26] and references therein. In [24], it was concluded that for the considered problem class, Magnus-type integrators used in conjunction with a Lanczos approach excel over splitting or partitioned Runge-Kutta methods.

The main objective of the present work is to construct and analyze defect-based *a posteriori* error estimators for Magnus-type integrators; for the purpose of comparison, widely used classical Magnus integrators are considered as well. Although only symmetric schemes appear in this paper, our considerations are fully general. We explicitly give the proof details for the second order exponential midpoint rule, which were also verified by computer algebra. Working out the detailed expressions for higher order methods is not feasible without massive use of such technology, which is beyond the scope of the present work. We stress, however, that this pertains only to theoretical aspects and does not negatively influence the construction and practical use of the resulting error estimators.

Notation for commutators. We employ the common denotation $\mathrm{ad}_\Omega(A) := [\Omega, A] = \Omega A - A\Omega$ for the commutator of two matrices $\Omega, A \in \mathbb{C}^{n\times n}$, and the symbol ad^k refers to repeated application of the commutation operator,

$$\begin{aligned} &\mathrm{ad}_\Omega^0(A) = A,\\ &\mathrm{ad}_\Omega^m(A) = \big[\Omega, \mathrm{ad}_\Omega^{m-1}(A)\big] = \Omega\,\mathrm{ad}_\Omega^{m-1}(A) - \mathrm{ad}_\Omega^{m-1}(A)\,\Omega, \quad m \in \mathbb{N}. \end{aligned} \tag{1.3}$$

2. Magnus-type integrators

We consider Magnus-type one-step methods for the approximation of (1.1) on a time grid $(t_0, t_1, \dots, t_n, \dots)$,

$$\psi_{n+1} = \mathcal{S}(\tau_n; t_n)\,\psi_n \approx \psi(t_{n+1}) = \mathcal{E}(\tau_n; t_n)\,\psi(t_n), \quad \tau_n = t_{n+1} - t_n, \quad n = 0, 1, 2, \dots.$$

In the sequel, for describing the particular schemes under consideration, we use a simplified notation and consider a single step starting from $t = t_0$ with stepsize τ,

$$\psi_1 = \mathcal{S}(\tau; t_0)\,\psi_0 \approx \psi(t_0 + \tau). \tag{2.1}$$

Furthermore, in order to avoid unnecessary overloading of notation, we suppress the dependence on t_0 of "internal" objects involved in the definition of the integrators. Only the dependence on the stepsize τ is indicated; see for instance (2.2) below.

Commutator-free Magnus-type (CFM) integrators. We first focus on higher-order commutator-free Magnus-type integrators [13]. These approximate the exact flow in terms of products of exponentials of linear combinations of the system matrix evaluated at different times, avoiding evaluation and storage of commutators.

A high-order CFM scheme is thus defined by (2.1), with

$$\begin{aligned} &\mathcal{S}(\tau; t_0) = \mathcal{S}_J(\tau)\cdots\mathcal{S}_1(\tau) = \mathrm{e}^{\Omega_J(\tau)}\,\cdots\,\mathrm{e}^{\Omega_1(\tau)}, \qquad \Omega_j(\tau) = \tau B_j(\tau), \quad j = 1, \dots, J,\\ &B_j(\tau) = \sum_{k=1}^{K} a_{jk}\,A_k(\tau), \qquad A_k(\tau) = A(t_0 + c_k\tau), \end{aligned} \tag{2.2}$$

where the coefficients a_{jk}, c_k are chosen such that the method realizes a certain convergence order p. For convenience, we collect the coefficients in

$$c = (c_1, \dots, c_K) \in [0,1]^K, \qquad a = \begin{pmatrix} a_{11} & \dots & a_{1K}\\ \vdots & \ddots & \vdots\\ a_{J1} & \dots & a_{JK} \end{pmatrix} \in \mathbb{R}^{J\times K}. \tag{2.3}$$

Examples of symmetric CFM integrators.

(i) The second-order exponential midpoint scheme ($p = 2$), given by

$$J = 1, \quad K = 1, \qquad c = \tfrac{1}{2}, \quad a = 1,$$

is a simple instance of a Magnus-type integrator. Thus,

$$\mathcal{S}(\tau; t_0) = \mathrm{e}^{\tau A(t_0 + \frac{\tau}{2})}. \tag{2.4}$$

(ii) A fourth-order commutator-free integrator ($p = 4$) based on two Gaussian nodes and comprising two matrix exponentials is defined by

$$J = 2, \quad K = 2, \qquad c = \left(\tfrac{1}{2} - \tfrac{\sqrt{3}}{6}, \tfrac{1}{2} + \tfrac{\sqrt{3}}{6}\right), \quad a = \begin{pmatrix} \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} - \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} \end{pmatrix}. \tag{2.5a}$$

(iii) An optimized fourth-order scheme ($p = 4$) from [1] is

$$J = 3, \quad K = 3, \qquad c = \begin{pmatrix} \frac{1}{2} - \frac{\sqrt{15}}{10} \\ \frac{1}{2} \\ \frac{1}{2} + \frac{\sqrt{15}}{10} \end{pmatrix}, \quad a = \begin{pmatrix} \frac{37}{240} + \frac{10}{87}\frac{\sqrt{15}}{3} & -\frac{1}{30} & \frac{37}{240} - \frac{10}{87}\frac{\sqrt{15}}{3} \\ -\frac{11}{360} & \frac{23}{45} & -\frac{11}{360} \\ \frac{37}{240} - \frac{10}{87}\frac{\sqrt{15}}{3} & -\frac{1}{30} & \frac{37}{240} + \frac{10}{87}\frac{\sqrt{15}}{3} \end{pmatrix}. \tag{2.5b}$$

(iv) A sixth-order commutator-free integrator ($p = 6$) based on three Gaussian nodes and comprising six matrix exponentials is given by

$$J = 6, \quad K = 3, \qquad c = \left(\tfrac{1}{2} - \tfrac{\sqrt{15}}{10}, \tfrac{1}{2}, \tfrac{1}{2} + \tfrac{\sqrt{15}}{10}\right),$$
$$a = \begin{pmatrix} 0.2158389969757678 & -0.0767179645915514 & 0.0208789676157837 \\ -0.0808977963208530 & -0.1787472175371576 & 0.0322633664310473 \\ 0.1806284600558301 & 0.4776874043509313 & -0.0909342169797981 \\ -0.0909342169797981 & 0.4776874043509313 & 0.1806284600558301 \\ 0.0322633664310473 & -0.1787472175371576 & -0.0808977963208530 \\ 0.0208789676157837 & -0.0767179645915514 & 0.2158389969757678 \end{pmatrix}, \tag{2.6}$$

see [1].

Classical Magnus integrators. A different, indeed the more classical, approach to the approximation of (1.1) is directly based on the Magnus expansion [27]: The solution to a time-dependent system (1.1) can be represented by

$$\psi(t_0 + \tau) = \mathcal{E}(\tau; t_0)\psi_0 = \mathrm{e}^{\mathbf{\Omega}(\tau)}\psi_0, \tag{2.7a}$$

where $\mathbf{\Omega}(\tau)$ satisfies

$$\mathbf{\Omega}'(\tau) = \sum_{k \geq 0} \frac{B_k}{k!} \, \mathrm{ad}^k_{\mathbf{\Omega}(\tau)}(A(t_0 + \tau)), \quad \mathbf{\Omega}(0) = 0, \tag{2.7b}$$

with the Bernoulli numbers B_k.

Classical Magnus integrators rely on appropriate truncation of the Magnus expansion (2.7b) and suitable approximation $\Omega(\tau)$ to the arising multi-dimensional integral representation for $\mathbf{\Omega}(\tau)$ by numerical quadrature, and defining ψ_1 by (2.1) with

$$\mathcal{S}(\tau; t_0) = \mathrm{e}^{\Omega(\tau)} \approx \mathrm{e}^{\mathbf{\Omega}(\tau)}. \tag{2.8}$$

A detailed exposition on this approach is given for example in [10] and in [16].

This type of integrator is, in general, considered as computationally expensive due to the requirement to compute and store commutators of large matrices. For problems of a particular structure, however, as in the semiclassical regime, or when commutators turn out to be of higher order $O(\tau^k)$ than $O(1)$ as expected generically, this approach may excel over the commutator-free methods, see [1, 7].

Examples of classical symmetric Magnus integrators. Again we denote

$$A_k(\tau) = A(t_0 + c_k\tau), \tag{2.9}$$

with a set of nodes defined by $c = (c_1, \dots, c_K) \in [0,1]^K$.

(i) The exponential midpoint scheme (2.4) (order $p = 2$) is also a classical Magnus integrator, with $K = 1$ and

$$c = \tfrac{1}{2}, \quad \Omega(\tau) = \tau A_1(\tau). \tag{2.10}$$

(ii) A commonly used fourth-order Magnus integrator ($p = 4$) is based on two Gaussian nodes, with $K = 2$ and

$$c = \Big(\tfrac{1}{2} - \tfrac{\sqrt{3}}{6}, \tfrac{1}{2} + \tfrac{\sqrt{3}}{6}\Big), \quad \Omega(\tau) = \tfrac{1}{2}\tau\big(A_1(\tau) + A_2(\tau)\big) - \tfrac{\sqrt{3}}{12}\,\tau^2\big[A_1(\tau), A_2(\tau)\big]. \tag{2.11}$$

(iii) A sixth-order Magnus integrator ($p = 6$) based on three Gaussian nodes ($K = 3$) is given by

$$\begin{aligned}
c &= \Big(\tfrac{1}{2} - \tfrac{\sqrt{15}}{10}, \tfrac{1}{2}, \tfrac{1}{2} + \tfrac{\sqrt{15}}{10}\Big),\\
\alpha_1(\tau) &= \tau A_2(\tau), \quad \alpha_2(\tau) = \tfrac{\sqrt{15}}{3}\,\tau\big(A_3(\tau) - A_1(\tau)\big), \quad \alpha_3(\tau) = \tfrac{10}{3}\tau\big(A_1(\tau) - 2\,A_2(\tau) + A_3(\tau)\big),\\
C_1(\tau) &= \big[\alpha_1(\tau), \alpha_2(\tau)\big], \quad C_2(\tau) = -\tfrac{1}{60}\big[\alpha_1(\tau), 2\,\alpha_3(\tau) + C_1(\tau)\big],\\
\Omega(\tau) &= \alpha_1(\tau) + \tfrac{1}{12}\,\alpha_3(\tau) + \tfrac{1}{240}\big[-20\,\alpha_1(\tau) - \alpha_3(\tau) + C_1(\tau), \alpha_2(\tau) + C_2(\tau)\big],
\end{aligned} \tag{2.12}$$

adhering to the notation from equation (251) of [10].

3. Defect-based *a posteriori* local error estimators

The local error of (2.1) is

$$\psi_1 - \psi(t_0 + \tau) = \mathcal{L}(\tau; t_0)\,\psi_0, \tag{3.1a}$$

with the local error operator

$$\mathcal{L}(\tau; t_0) = \mathcal{S}(\tau; t_0) - \mathcal{E}(\tau; t_0). \tag{3.1b}$$

We aim for designing asymptotically correct computable estimators

$$\widetilde{\mathcal{L}}(\tau; t_0)\,\psi_0 \approx \mathcal{L}(\tau; t_0)\,\psi_0$$

for the local error of CFM and classical Magnus integrators, based on the notion of the defect of the numerical approximation. The idea is related to [4, 5].

Remark 3.1. In the remainder of this section, $\mathcal{L}(\tau; t_0)$ is simply called the local error. The associated defect operator $\mathcal{D}(\tau; t_0)$ defined in (3.3) below is simply called the defect. The error estimator $\widetilde{\mathcal{L}}(\tau; t_0)\,\psi_0$ will be based on (approximate) evaluation of the defect at ψ_0.

3.1. Basic idea of the construction

We proceed from the fact that a one-step approximation (2.1) of order p is characterized by the property $\mathcal{L}(\tau;t_0)=\mathcal{O}(\tau^{p+1})$, or equivalently, $\mathcal{L}(0;t_0)=0$ and

$$\tfrac{\mathrm{d}^q}{\mathrm{d}\tau^q}\mathcal{L}(\tau;t_0)\big|_{\tau=0}=0,\quad q=1,\ldots,p. \tag{3.2}$$

With the defect

$$\mathcal{D}(\tau;t_0)=\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}(\tau;t_0)-A(t_0+\tau)\,\mathcal{S}(\tau;t_0), \tag{3.3}$$

the local error, as a function of τ, is the solution of

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{L}(\tau;t_0)=A(t_0+\tau)\,\mathcal{L}(\tau;t_0)+\mathcal{D}(\tau;t_0),\qquad \mathcal{L}(0;t_0)=0, \tag{3.4a}$$

whence by the variation-of-constants formula,[4]

$$\mathcal{L}(\tau;t_0)=\int_0^\tau \Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0)\,\mathrm{d}\sigma=:\int_0^\tau \widehat{\mathcal{D}}(\sigma;t_0)\,\mathrm{d}\sigma, \tag{3.4b}$$

with

$$\Pi(\tau,\sigma)=\mathcal{E}(\tau;t_0)\,\mathcal{E}(-\sigma;t_0+\sigma)=\mathcal{E}(\tau-\sigma;t_0+\sigma),\quad \Pi(\tau,\tau)=\mathrm{Id}.$$

Repeated differentiation of (3.4a) gives

$$\tfrac{\mathrm{d}^q}{\mathrm{d}\tau^q}\mathcal{L}(\tau;t_0)=\sum_{k=0}^{q-1}\tbinom{q-1}{k}\,\tfrac{\mathrm{d}^{q-1-k}}{\mathrm{d}\tau^{q-1-k}}A(t_0+\tau)\,\tfrac{\mathrm{d}^k}{\mathrm{d}\tau^k}\mathcal{L}^{(k)}(\tau)+\tfrac{\mathrm{d}^{q-1}}{\mathrm{d}\tau^{q-1}}\mathcal{D}(\tau;t_0),$$

thus the relations (3.2) are equivalent to

$$\tfrac{\mathrm{d}^q}{\mathrm{d}\tau^q}\mathcal{D}(\tau;t_0)\big|_{\tau=0}=0,\quad q=0,\ldots,p-1. \tag{3.5}$$

Therefore the integrand

$$\widehat{\mathcal{D}}(\sigma;t_0)=\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0) \tag{3.6a}$$

in (3.4b) also satisfies

$$\tfrac{\mathrm{d}^q}{\mathrm{d}\sigma^q}\widehat{\mathcal{D}}(\sigma;t_0)\big|_{\sigma=0}=0,\quad q=0,\ldots,p-1. \tag{3.6b}$$

For the integral in (3.4b) we now consider an approximation of order $\mathcal{O}(\tau^{p+2})$ based on Taylor expansion,

$$\begin{aligned}\mathcal{L}(\tau;t_0)&=\int_0^\tau \widehat{\mathcal{D}}(\sigma;t_0)\,\mathrm{d}\sigma\approx\int_0^\tau \tfrac{\sigma^p}{p!}\widehat{\mathcal{D}}^{(p)}(0;t_0)\,\mathrm{d}\sigma=\tfrac{\tau^{p+1}}{(p+1)!}\widehat{\mathcal{D}}^{(p)}(0;t_0)\\ &\approx\tfrac{\tau}{p+1}\widehat{\mathcal{D}}(\tau;t_0)=\tfrac{\tau}{p+1}\,\Pi(\tau,\tau)\,\mathcal{D}(\tau;t_0)=\tfrac{\tau}{p+1}\mathcal{D}(\tau;t_0).\end{aligned} \tag{3.7a}$$

Here, "$\approx$" means asymptotic approximation at the level $\mathcal{O}(\tau^{p+2})$, where the approximation error depends on $\frac{\mathrm{d}^{p+1}}{\mathrm{d}\sigma^{p+1}}\widehat{\mathcal{D}}(\sigma;t_0)$. The local error estimate

$$\tfrac{\tau}{p+1}\mathcal{D}(\tau;t_0)=\mathcal{L}(\tau;t_0)+\mathcal{O}(\tau^{p+2})$$

defined by (3.7a) involves a single evaluation of the defect $\mathcal{D}(\tau;t_0)$ for the given stepsize τ. The derivative $\frac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}(\tau;t_0)$ involved in the definition (3.3) of $\mathcal{D}(\tau;t_0)$ is not directly computable but, as shown below, it can be expressed in a derivative-free way, and this enables a computable, asymptotically correct approximation

$$\widetilde{\mathcal{D}}(\tau;t_0)=\mathcal{D}(\tau;t_0)+\mathcal{O}(\tau^{p+1}). \tag{3.7b}$$

[4]The two-parameter matrix family $\Pi(\tau,\sigma)$ is called an evolution system associated with $A(t)$. The representation (3.4b) can be interpreted as a consequence of the general nonlinear variation-of-constants formula, also called the Gröbner-Alekseev Lemma, see Theorem I.14.5 of [17].

The resulting practical error estimator is denoted by

$$\widetilde{\mathcal{L}}(\tau;t_0) = \tfrac{\tau}{p+1}\widetilde{\mathcal{D}}(\tau;t_0) = \mathcal{L}(\tau;t_0) + \mathcal{O}(\tau^{p+2}). \tag{3.7c}$$

The error of this approximation will be analyzed in more detail in Section 4.

In view of the form of the schemes of types (2.2) or (2.8) considered here, $\mathcal{D}(\tau;t_0)$ contains terms of the type $\frac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\Omega(\tau)}$, in particular with $\Omega(\tau)$ of the form $\Omega(\tau) = \tau B(\tau)$. Therefore we first collect representations for derivatives of matrix exponentials, for the purpose of constructing derivative-free approximations (3.7b).

3.2. Derivatives of matrix exponentials

Fréhet derivative of the matrix exponential. An induction argument shows that the Fréchet derivative of matrix powers Ω^k with respect to $\Omega \in \mathbb{C}^{d\times d}$, evaluated at $V \in \mathbb{C}^{d\times d}$, is given by

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\Omega^m\big)(V) = \sum_{k=0}^{m} \Omega^{m-1-k}\, V\, \Omega^k = \sum_{k=0}^{m-1} \tbinom{m}{k+1}\, \mathrm{ad}_\Omega^k(V)\, \Omega^{m-1-k}, \qquad m \in \mathbb{N},$$

see Section III.4, (4.3) of [16]. This implies that the Fréchet derivative of

$$\mathrm{e}^\Omega = \sum_{m\ge 0} \tfrac{1}{m!}\, \Omega^m$$

takes the form

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\mathrm{e}^\Omega\big)(V) = \sum_{m\ge 0} \tfrac{1}{(m+1)!}\, \mathrm{ad}_\Omega^m(V)\, \mathrm{e}^\Omega, \tag{3.8a}$$

see Section III.4, Lemma 1 of [16].

An alternative representation even more useful for our purpose is given by the integral formula (see [19], Sect. 10.2, (10.15))[5]

$$\big(\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\mathrm{e}^\Omega\big)(V) = \int_0^1 \mathrm{e}^{s\Omega}\, V\, \mathrm{e}^{-s\Omega}\, \mathrm{d}s \cdot \mathrm{e}^\Omega. \tag{3.8b}$$

Time derivative. For a given time-dependent matrix $\Omega = \Omega(\tau)$, the matrix-valued function $\mathrm{e}^{\Omega(\tau)}$ satisfies a linear differential equation. In particular, (3.8a) implies[6]

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\Omega(\tau)} = \big(\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\mathrm{e}^\Omega\big)\big|_{\Omega(\tau)}(\Omega'(\tau)) = \Gamma(\tau)\, \mathrm{e}^{\Omega(\tau)}, \quad \text{with} \quad \Gamma(\tau) = \sum_{m\ge 0} \tfrac{1}{(m+1)!}\, \mathrm{ad}_{\Omega(\tau)}^m(\Omega'(\tau)).$$

For a time-dependent matrix of the form appearing in the integrators considered,

$$\Omega(\tau) = \tau B(\tau), \tag{3.9}$$

we have $\Omega'(\tau) = B(\tau) + \tau B'(\tau)$ and

$$\mathrm{ad}_{\Omega(\tau)}^m(\Omega'(\tau)) = \tau^{m+1}\, \mathrm{ad}_{B(\tau)}^m(B'(\tau)), \quad m \in \mathbb{N},$$

which implies

$$\begin{aligned} &\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)} = \Gamma(\tau)\, \mathrm{e}^{\tau B(\tau)}, \\ &\text{with} \quad \Gamma(\tau) = B(\tau) + \sum_{m\ge 0} \tfrac{1}{(m+1)!}\tau^{m+1}\mathrm{ad}_{B(\tau)}^m(B'(\tau)) \\ &\qquad\qquad = B(\tau) + \tau B'(\tau) + \tfrac{1}{2}\tau^2[B(\tau), B'(\tau)] + \tfrac{1}{6}\tau^3[B(\tau),[B(\tau),B'(\tau)]] + \dots. \end{aligned} \tag{3.10a}$$

[5] The integrand in this formula is also denoted by $\mathrm{Ad}_{\mathrm{e}^{s\Omega}}(V)$ in the literature [16], but since this operator is not used again later in this paper, this notation is not called for.

[6] For $\Omega(\tau) = \boldsymbol{\Omega}(\tau)$ from (2.7) we have $\Gamma(\tau) = A(t_0+\tau)$.

A computable approximation for the time derivative $\frac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)}$ with error $\mathcal{O}(\tau^{p+1})$ is obtained by truncating the sum in (3.10a), *i.e.*,

$$\widetilde{\Gamma}(\tau)\,\mathrm{e}^{\tau B(\tau)} = \tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)} + \mathcal{O}(\tau^{p+1}), \quad \text{with} \quad \widetilde{\Gamma}(\tau) = \sum_{m=0}^{p} \tfrac{1}{m!}\tau^m\,\mathrm{ad}_{B(\tau)}^m(B'(\tau)). \tag{3.10b}$$

Alternatively, for $\Omega(\tau)$ of the form (3.9), the representation (3.8b) together with the substitution $\tau s = \sigma$ gives[7]

$$\begin{aligned} &\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)} = \Gamma(\tau)\,\mathrm{e}^{\tau B(\tau)}, \\ &\text{with} \quad \Gamma(\tau) = B(\tau) + \int_0^\tau F(\sigma;\tau)\,\mathrm{d}\sigma, \quad F(\sigma;\tau) = \mathrm{e}^{\sigma B(\tau)}\,B'(\tau)\,\mathrm{e}^{-\sigma B(\tau)}, \end{aligned} \tag{3.11a}$$

and replacing the integral in (3.11a) by a quadrature formula of order p also leads to a computable approximation for the time derivative $\frac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)}$ in the form

$$\widetilde{\Gamma}(\tau)\,\mathrm{e}^{\tau B(\tau)} = \tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)} + \mathcal{O}(\tau^{p+1}), \quad \text{where} \quad \widetilde{\Gamma}(\tau) \;=\; \text{quadrature approximation of } \Gamma(\tau) \text{ with error } \mathcal{O}(\tau^{p+1}). \tag{3.11b}$$

Here one may apply conventional interpolatory quadrature or, as a better choice avoiding evitable additional evaluation of exponentials, Hermite-type quadrature involving evaluations of a number of derivatives of the integrand $F(\sigma;\tau)$ at $\sigma = 0$ or $\sigma = \tau$, which depend on commutators $\mathrm{ad}_{B(\tau)}^m(B'(\tau))$. See (3.18) below for a typical example.

The special case where only evaluations of the integrand at $\sigma = 0$ are used, corresponds to the truncated expansion $\widetilde{\Gamma}(\tau)$ from (3.10b). We may call this "Taylor quadrature", since it is based on Taylor expansion of the integrand w.r.t. σ for given τ; we denote it by $T_p(F,0,\tau)$. For a typical example, see (3.17) below.

On the basis of such an approximation $\widetilde{\Gamma}(\tau) \approx \Gamma(\tau) \approx A(t_0+\tau)$, computable asymptotically correct approximations $\widetilde{\mathcal{D}}(\tau;t_0)$ of the defect $\mathcal{D}(\tau;t_0)$ defined in (3.3) can be constructed. In the sequel we describe some variants.

3.3. Local error estimators for CFM integrators.

For CFM integrators (2.2), the defect is given by (3.3),

$$\begin{aligned} \mathcal{D}(\tau;t_0) &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\mathcal{S}(\tau;t_0) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0) \\ &= \big(\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}_J(\tau)\big)\,\mathcal{S}_{J-1}(\tau)\cdots\mathcal{S}_1(\tau) \;+\; \ldots \;+\; \mathcal{S}_J(\tau)\cdots\mathcal{S}_2(\tau)\,\big(\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}_1(\tau)\big) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0) \\ &= \Gamma_J(\tau)\,\mathcal{S}_J(\tau)\,\mathcal{S}_{J-1}(\tau)\cdots\mathcal{S}_1(\tau) \;+\; \ldots \;+\; \mathcal{S}_J(\tau)\cdots\mathcal{S}_2(\tau)\,\Gamma_1(\tau)\,\mathcal{S}_1(\tau) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0), \end{aligned}$$

with $\mathcal{S}_j(\tau) = \mathrm{e}^{\Omega_j(\tau)} = \mathrm{e}^{\tau B_j(\tau)}$, and $\widetilde{\Gamma}_j$ related to B_j as in (3.10a). An asymptotically correct, computable approximation

$$\begin{aligned} \widetilde{\mathcal{D}}(\tau;t_0) &= \widetilde{\Gamma}_J(\tau)\,\mathcal{S}_J(\tau)\,\mathcal{S}_{J-1}(\tau)\cdots\mathcal{S}_1(\tau) \;+\; \ldots \;+\; \mathcal{S}_J(\tau)\cdots\mathcal{S}_2(\tau)\,\widetilde{\Gamma}_1(\tau)\,\mathcal{S}_1(\tau) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0) \\ &= \mathcal{D}(\tau;t_0) + \mathcal{O}(\tau^{p+1}) \end{aligned}$$

is obtained by approximating, for $j = 1,\ldots,J$, the $\Gamma_j(\tau)$ according to (3.10) or (3.11). This leads to different approximations $\widetilde{\Gamma}_j(\tau)$ for the $\Gamma_j(\tau)$ and corresponding defect approximations $\widetilde{\mathcal{D}}(\tau;t_0)$ and local error estimators $\widetilde{\mathcal{L}}(\tau;t_0)$, see (3.7c).

(i) Second-order exponential midpoint scheme (2.4): Here, $J = 1$ and $\mathcal{S}(\tau;t_0) = \mathcal{S}_1(\tau) = \mathrm{e}^{\tau B(\tau)}$ with $B(\tau) = B_1(\tau) = A(t_0 + \frac{\tau}{2})$. Thus,

$$\widetilde{\mathcal{D}}(\tau;t_0) = \widetilde{\Gamma}(\tau)\,\mathcal{S}(\tau;t_0) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0). \tag{3.12}$$

[7] In some references, like III.4.5 of [16], $\Gamma(\tau)$ is denoted by $d\exp_{B(\tau)}^{-1}(B'(\tau))$, we choose a more compact notation, however.

Using Taylor quadrature (3.10b) with $p = 2$, *i.e.*,

$$\widetilde{\Gamma}(\tau) = B(\tau) + \tau B'(\tau) + \tfrac{1}{2}\tau^2[B(\tau), B'(\tau)],$$

(3.12) takes the form

$$\begin{aligned}\widetilde{\mathcal{D}}(\tau; t_0) &= \big(B(\tau) + \tau B'(\tau) + \tfrac{1}{2}\tau^2[B(\tau), B'(\tau)] - A(t_0+\tau)\big)\,\mathcal{S}(\tau; t_0)\\ &= \big(A(t_0+\tfrac{\tau}{2}) + \tfrac{1}{2}\tau A'(t_0+\tfrac{\tau}{2}) + \tfrac{1}{4}\tau^2[A(t_0+\tfrac{\tau}{2}), A'(t_0+\tfrac{\tau}{2})] - A(t_0+\tau)\big)\,\mathcal{S}(\tau; t_0).\end{aligned} \tag{3.13a}$$

Provided that evaluation of A'' is available, another asymptotically correct simplification is

$$\widetilde{\mathcal{D}}(\tau; t_0) = \big(-\tfrac{1}{8}\tau^2\, A''(t_0+\tau) + \tfrac{1}{4}\tau^2\,[A(t_0+\tau), A'(t_0+\tau)]\big)\,\mathcal{S}(\tau; t_0). \tag{3.13b}$$

Application of $\widetilde{\mathcal{D}}(\tau; t_0)$ to ψ_0 does not require evaluation of an additional matrix exponential. For instance, in practice application of (3.13b) means: Compute

$$\widetilde{\mathcal{D}}(\tau; t_0)\psi_0 = \big(-\tfrac{1}{8}\tau^2\, A''(t_0+\tau) + \tfrac{1}{4}\tau^2\,[A(t_0+\tau), A'(t_0+\tau)]\big)\,\psi_1,$$

since $\mathcal{S}(\tau; t_0)\,\psi_0 = \psi_1$.

As an alternative, we approximate the integral representation of the type (3.11a) for $\Gamma(\tau)$ using the second-order trapezoidal quadrature,

$$\int_0^\tau F(\sigma; \tau)\,\mathrm{d}\sigma \approx Q_2(F, 0, \tau) = \tfrac{1}{2}\tau\big(F(0; \tau) + F(\tau; \tau)\big), \tag{3.14}$$

with $F(\sigma; \tau) = \mathrm{e}^{\sigma B(\tau)}\, B'(\tau)\, \mathrm{e}^{-\sigma B(\tau)}$ as in (3.11a). This gives the approximation

$$\widetilde{\Gamma}(\tau) = B(\tau) + \tfrac{1}{2}\tau\big(B'(\tau) + \mathrm{e}^{\tau B(\tau)} B'(\tau)\,\mathrm{e}^{-\tau B(\tau)}\big).$$

Then, (3.12) takes the form

$$\begin{aligned}\widetilde{\mathcal{D}}(\tau; t_0) &= \big(B(\tau) + \tfrac{1}{2}\tau(B'(\tau) + \mathrm{e}^{\tau B(\tau)} B'(\tau)\,\mathrm{e}^{-\tau B(\tau)}) - A(t_0+\tau)\big)\,\mathcal{S}(\tau; t_0)\\ &= \big(B(\tau) + \tfrac{1}{2}\tau B'(\tau) - A(t_0+\tau)\big)\,\mathcal{S}(\tau; t_0) + \tfrac{1}{2}\tau\,\mathcal{S}(\tau; t_0)\,B'(\tau)\\ &= \big(A(t_0+\tfrac{\tau}{2}) + \tfrac{1}{4}\tau A'(t_0+\tfrac{\tau}{2}) - A(t_0+\tau)\big)\,\mathcal{S}(\tau; t_0) + \tfrac{1}{4}\tau\,\mathcal{S}(\tau; t_0)\,A'(t_0+\tfrac{\tau}{2}).\end{aligned} \tag{3.15}$$

This involves evaluation of one additional matrix exponential, namely $\mathcal{S}(\tau; t_0)A'(t_0+\tfrac{\tau}{2})\,\psi_0$.

(ii) Fourth-order scheme of the type (2.5a): Here, $J = 2$ and $\mathcal{S}(\tau; t_0) = \mathcal{S}_2(\tau)\,\mathcal{S}_1(\tau) = \mathrm{e}^{\tau B_2(\tau)}\,\mathrm{e}^{\tau B_1(\tau)}$. Thus,

$$\widetilde{\mathcal{D}}(\tau; t_0) = \widetilde{\Gamma}_2(\tau)\,\mathcal{S}_2(\tau)\,\mathcal{S}_1(\tau) + \mathcal{S}_2(\tau)\,\widetilde{\Gamma}_1(\tau)\,\mathcal{S}_1(\tau) - A(t_0+\tau)\,\mathcal{S}(\tau; t_0). \tag{3.16}$$

Using Taylor quadrature (3.10b) with $p = 4$, *i.e.*,

$$\begin{aligned}\widetilde{\Gamma}_j(\tau) &= B_j(\tau) + \tau B_j'(\tau) + \tfrac{1}{2}\tau^2[B_j(\tau), B_j'(\tau)] + \tfrac{1}{6}\tau^3[B_j(\tau), [B_j(\tau), B_j'(\tau)]]\\ &\quad + \tfrac{1}{24}\tau^4[B_j(\tau), [B_j(\tau), [B_j(\tau), B_j'(\tau)]]], \quad j = 1, 2,\end{aligned} \tag{3.17}$$

results in evaluation of $\widetilde{\mathcal{D}}(\tau; t_0)$ according to (3.16) requiring the evaluation of one additional matrix exponential, namely $\mathcal{S}_2(\tau)\widetilde{\Gamma}_1(\tau)\,\mathcal{S}_1(\tau)\,\psi_0$, provided the intermediate value $\mathcal{S}_1(\tau)\,\psi_0$ is stored.

As an alternative, we consider the fourth-order modified trapezoidal quadrature of Hermite type,

$$\int_0^\tau F(\sigma; \tau)\,\mathrm{d}\sigma \approx Q_4(F, 0, \tau) = \tfrac{1}{2}\tau\big(F(0; \tau) + F(\tau; \tau)\big) + \tfrac{1}{12}\tau^2\Big(\tfrac{\partial}{\partial\sigma}F(\sigma; \tau)\big|_{\sigma=0} - \tfrac{\partial}{\partial\sigma}F(\sigma; \tau)\big|_{\sigma=\tau}\Big). \tag{3.18}$$

For $F(\sigma;\tau) = \mathrm{e}^{\sigma B_j(\tau)}\, B_j'(\tau)\, \mathrm{e}^{-\sigma B_j(\tau)}$ as in (3.11a) we have

$$\tfrac{\partial}{\partial\sigma} F(\sigma;\tau)\big|_{\sigma=0} = [B_j(\tau), B_j'(\tau)], \quad \tfrac{\partial}{\partial\sigma} F(\sigma;\tau)\big|_{\sigma=\tau} = \mathrm{e}^{\tau B_j(\tau)}\,[B_j(\tau), B_j'(\tau)]\,\mathrm{e}^{-\tau B_j(\tau)}.$$

For the integral representation of the type (3.11a) for the $\Gamma_j(\tau)$ this gives, for $j = 1, 2$,

$$\begin{aligned}\widetilde{\Gamma}_j(\tau) = B_j(\tau) &+ \tfrac{1}{2}\tau\big(B_j'(\tau) + \mathrm{e}^{\tau B_j(\tau)} B_j'(\tau)\,\mathrm{e}^{-\tau B_j(\tau)}\big)\\ &+ \tfrac{1}{12}\tau^2\big([B_j(\tau), B_j'(\tau)] - \mathrm{e}^{\tau B_j(\tau)}\,[B_j(\tau), B_j'(\tau)]\,\mathrm{e}^{-\tau B_j(\tau)}\big).\end{aligned} \tag{3.19a}$$

Thus, with $\mathcal{S}_j(\tau) = \mathrm{e}^{\tau B_j(\tau)}$,

$$\widetilde{\Gamma}_j(\tau)\,\mathcal{S}_j(\tau) = C_j^+(\tau)\,\mathcal{S}_j(\tau) + \mathcal{S}_j(\tau)\,C_j^-(\tau), \quad C_j^\pm(\tau) = \tfrac{1}{2}\big(B_j(\tau) + \tau B_j'(\tau)\big) \pm \tfrac{1}{12}\tau^2[B_j(\tau), B_j'(\tau)]. \tag{3.19b}$$

Then, (3.16) takes the form

$$\widetilde{\mathcal{D}}(\tau;t_0) = \big(C_2^+(\tau) - A(t_0+\tau)\big)\,\mathcal{S}_2(\tau)\,\mathcal{S}_1(\tau) + \mathcal{S}_2(\tau)\Big(\big(C_1^+(\tau) + C_2^-(\tau)\big)\,\mathcal{S}_1(\tau) + \mathcal{S}_1(\tau)\,C_1^-(\tau)\Big). \tag{3.20}$$

This requires the evaluation of two additional exponentials (again provided the intermediate value $\mathcal{S}_1(\tau)\,\psi_0$ is stored), but only first-order commutator expressions are involved in the evaluation of $C_j^\pm(\tau)$. Again, the basic scheme and the defect are evaluated in parallel.

(iii) For higher-order schemes as for instance (2.6), the evaluation of the defect of course becomes more expensive. For schemes of order 6, for instance, applying the sixth order Hermite-type quadrature

$$\begin{aligned}\int_0^\tau F(\sigma;\tau)\,\mathrm{d}\sigma \approx Q_6(F,0,\tau) = \tfrac{1}{2}\tau(F(0;\tau) + F(\tau;\tau)) &+ \tfrac{1}{10}\tau^2\Big(\tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=0} - \tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=\tau}\Big)\\ &+ \tfrac{1}{120}\tau^3\Big(\tfrac{\partial^2}{\partial\sigma^2}F(\sigma;\tau)\big|_{\sigma=0} + \tfrac{\partial^2}{\partial\sigma^2}F(\sigma;\tau)\big|_{\sigma=\tau}\Big),\end{aligned} \tag{3.21}$$

with $F(\sigma;\tau) = \mathrm{e}^{\sigma B_j(\tau)}\, B_j'(\tau)\,\mathrm{e}^{-\sigma B_j(\tau)}$ as before, and

$$\tfrac{\partial^2}{\partial\sigma^2} F(\sigma;\tau)\big|_{\sigma=0} = \mathrm{ad}^2_{B_j(\tau)}(B_j'(\tau)), \quad \tfrac{\partial^2}{\partial\sigma^2} F(\sigma;\tau)\big|_{\sigma=\tau} = \mathrm{e}^{\tau B_j(\tau)}\,\mathrm{ad}^2_{B_j(\tau)}(B_j'(\tau))\,\mathrm{e}^{-\tau B_j(\tau)},$$

is a reasonable option, and evaluation of $\mathcal{D}(\tau;t_0)$ is straightforward as for lower-order schemes. We give no further details here.

3.4. Local error estimators for classical Magnus integrators.

Classical Magnus integrators are of the form (2.8), where again $\Omega(\tau)$ is of the form $\tau B(\tau)$. Thus,

$$\begin{aligned}\mathcal{D}(\tau;t_0) &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\mathcal{S}(\tau;t_0) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0)\\ &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)} - A(t_0+\tau)\,\mathrm{e}^{\tau B(\tau)} = \Gamma(\tau)\,\mathrm{e}^{\tau B(\tau)} - A(t_0+\tau)\,\mathrm{e}^{\tau B(\tau)},\end{aligned} \tag{3.22}$$

which can be approximated on the basis of (3.10b) or (3.11b).

As an example we consider the fourth-order scheme defined by (2.11), where

$$B(\tau) = \tfrac{1}{2}\big(A(t_0+c_1\tau) + A(t_0+c_2\tau)\big) - \tfrac{\sqrt{3}}{12}\,\tau\,[A(t_0+c_1\tau), A(t_0+c_2\tau)],$$

with

$$\begin{aligned}B'(\tau) = &\tfrac{1}{2}\big(c_1 A'(t_0+c_1\tau) + c_2 A'(t_0+c_2\tau)\big)\\ &- \tfrac{\sqrt{3}}{12}\,[A(t_0+c_1\tau), A(t_0+c_2\tau)]\\ &- \tfrac{\sqrt{3}}{12}\,\tau\big(c_1\,[A'(t_0+c_1\tau), A(t_0+c_2\tau)] + c_2\,[A(t_0+c_1\tau), A'(t_0+c_2\tau)]\big).\end{aligned}$$

TABLE 1. Additional computational effort for error estimators.

	CFM estimator			Classical Magnus estimator		
p	Variant	ad^k	Additional exp	Variant	ad^k	Additional exp
2	(3.13)	$k=1$	0	(3.13)	$k=1$	0
	(3.15)	$k=0$	1	(3.15)	$k=0$	1
4	(3.17)	$k=3$	1	(3.24)	$k=3$	0
	(3.19)	$k=1$	2	(3.25)	$k=1$	1

Using Taylor quadrature (3.10b) with $p=4$ as in (3.17), *i.e.*,

$$\begin{aligned}\widetilde{\Gamma}(\tau) &= B(\tau)+\tau B'(\tau)+\tfrac{1}{2}\tau^2[B(\tau),B'(\tau)]+\tfrac{1}{6}\tau^3[B(\tau),[B(\tau),B'(\tau)]]\\ &\quad+\tfrac{1}{24}\tau^4[B(\tau),[B(\tau),[B(\tau),B'(\tau)]]],\end{aligned}$$

results in evaluation of $\widetilde{\mathcal{D}}(\tau;t_0)$ in the form

$$\widetilde{\mathcal{D}}(\tau;t_0)=\big(\widetilde{\Gamma}(\tau)-A(t_0+\tau)\big)\,\mathcal{S}(\tau;t_0), \tag{3.23}$$

without evaluation of an additional matrix exponential, but involving evaluation of nested commutators.

Alternatively, approximating the integral representation (3.11a) by the modified trapezoidal rule (3.18) gives the same expressions as in (3.19),

$$\begin{aligned}\widetilde{\Gamma}(\tau) &= B(\tau)+\tfrac{1}{2}\tau\big(B'(\tau)+\mathrm{e}^{\tau B(\tau)}B'(\tau)\,\mathrm{e}^{-\tau B(\tau)}\big)\\ &\qquad+\tfrac{1}{12}\tau^2\big([B(\tau),B'(\tau)]-\mathrm{e}^{\tau B(\tau)}\,[B(\tau),B'(\tau)]\,\mathrm{e}^{-\tau B(\tau)}\big),\end{aligned} \tag{3.24}$$

and, with $\mathcal{S}(\tau;t_0)=\mathrm{e}^{\tau B(\tau)}$,

$$\widetilde{\Gamma}(\tau)\,\mathcal{S}(\tau;t_0)=C^{+}(\tau)\,\mathcal{S}(\tau;t_0)+\mathcal{S}(\tau;t_0)\,C^{-}(\tau),\quad C^{\pm}(\tau)=\tfrac{1}{2}\big(B(\tau)+\tau B'(\tau)\big)\pm\tfrac{1}{12}\tau^2[B(\tau),B'(\tau)]. \tag{3.25}$$

Then, (3.22) takes the form

$$\widetilde{\mathcal{D}}(\tau;t_0)=\big(C^{+}(\tau)-A(t_0+\tau)\big)\,\mathcal{S}(\tau;t_0)+\mathcal{S}(\tau;t_0)\,C^{-}(\tau). \tag{3.26}$$

This requires evaluation of one additional exponential and a number of evaluations of commutators.

Remark: In [11], another way of estimating the local time-stepping error for classical Magnus integrators was discussed. A local extrapolation strategy explicitly resorting to the Baker–Campbell–Hausdorff formula [16] allows to construct error estimators by economically reusing evaluations of commutators and/or exponentials. Again a tradeoff between using more (nested) commutators or exponentials has to be taken into consideration, likewise as in our approach. In [11], an estimator for a classical Magnus integrator is for instance constructed without introducing an additional exponential, but at the cost of the computation of additional nested commutators. Our estimator (3.23) has precision $p+1$ and is thus asymptotically correct, while the estimator [11] is based on comparison with a method of lower order $p-2$.

In Table 1 we give an overview of the additional computational effort required by the different variants of error estimators for the cases $p=2$ and $p=4$, in terms of the degree of nested commutators involved and the number of additional exponentials which need to be evaluated.

4. Asymptotic analysis

By construction, for a scheme of order p all local error estimators $\widetilde{\mathcal{L}}(\tau;t_0) = \frac{\tau}{p+1}\,\widetilde{\mathcal{D}}(\tau;t_0)$ are asymptotically correct for $\tau \to 0$, *i.e.*, they satisfy (3.7c),

$$\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0) = \mathcal{O}(\tau^{p+2}). \tag{4.1}$$

In the following we provide a more precise characterization of the error of the error estimate, *i.e.*, of the deviation $\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)$, in the following sense.

- First of all, the $\mathcal{O}(\tau^{p+2})$ deviation (4.1) is influenced by two different contributions, caused by
  (i) approximation of the local error $\mathcal{L}(\tau;t_0)$ in terms of the exact defect $\mathcal{D}(\tau;t_0)$, see (3.7a),
  (ii) approximation of the defect $\mathcal{D}(\tau;t_0)$ by a computable approximation $\widetilde{\mathcal{D}}(\tau;t_0)$ via quadrature, see (3.7b) and Sections 3.3 & 3.4.
  For a discussion of these two contributions see Section 4.1.
- A more detailed analysis of the nature of these sources of error depends on the given scheme and type of error estimator at hand. We expect that certain commutator expressions involving higher derivatives of $A(t)$ enter the error constants behind (4.1). Without massive use of computer algebra, which is beyond the scope of the present work, working out the detailed expressions is not feasible. Therefore in Section 4.2 we confine ourselves to the case of the second-order exponential midpoint scheme.

4.1. Classification of terms influencing the deviation (4.1)

The approximation errors can be characterized as follows.

ad (i): The approximation (3.7a) can be interpreted as an Hermite-type quadrature for the local error integral (3.4b), involving only a single evaluation[8] of the defect $\mathcal{D}(\tau;t_0)$ (cf. [4, 5]). The corresponding quadrature error has the Peano representation

$$\tfrac{\tau}{p+1}\,\mathcal{D}(\tau;t_0) - \mathcal{L}(\tau;t_0) = \int_0^\tau K_{p+1}(\sigma)\,\tfrac{\mathrm{d}^{p+1}}{\mathrm{d}\sigma^{p+1}}\widehat{\mathcal{D}}(\sigma;t_0)\,\mathrm{d}\sigma, \quad \widehat{\mathcal{D}}(\sigma;t_0) = \Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0), \tag{4.2a}$$

with kernel

$$K_{p+1}(\sigma) = \frac{\sigma(\tau-\sigma)^p}{(p+1)!}\cdot \tag{4.2b}$$

ad (ii): Applying quadrature to integrals as in (3.11a), with integrands of the type

$$F(\sigma;\tau) = \mathrm{e}^{\sigma B(\tau)}\,B'(\tau)\,\mathrm{e}^{-\sigma B(\tau)},$$

results in $\widetilde{\mathcal{D}}(\tau;t_0) \approx \mathcal{D}(\tau;t_0)$. The Peano representations of the corresponding quadrature errors read as follows; here, derivatives of $F(\sigma;\tau)$ are to be understood as partial derivatives w.r.t. σ.

***p*-th order Taylor quadrature** (3.10b)**.**

$$\begin{aligned} T_p(F,0,\tau) - \int_0^\tau F(\sigma;\tau)\,\mathrm{d}\sigma &= \int_0^\tau -\tfrac{1}{p!}\,(\tau-\sigma)^p F^{(p)}(\sigma;\tau)\,\mathrm{d}\sigma \\ &= -\tfrac{1}{(p+1)!}\,\tau^{p+1}F^{(p)}(0;\tau) + \mathcal{O}(\tau^{p+2}), \end{aligned} \tag{4.3a}$$

with

$$F^{(p)}(\sigma;\tau) = \mathrm{e}^{\sigma B(\tau)}\,\mathrm{ad}^p_{B(\tau)}(B'(\tau))\,\mathrm{e}^{-\sigma B(\tau)}.$$

---

[8] This quadrature formula is based on higher-order Hermite interpolation and corresponding evaluations of $\frac{\mathrm{d}^q}{\mathrm{d}\tau^q}\mathcal{D}(\tau;t_0)\big|_{\tau=0}$, $q = 0,\ldots,p-1$, which vanish for a scheme of order p, see (3.5).

Second-order trapezoidal rule (3.14)**.**

$$Q_2(F,0,\tau) - \int_0^\tau F(\sigma;\tau)\,\mathrm{d}\sigma = \int_0^\tau \tfrac{1}{2}\,\sigma(\tau-\sigma)\,F''(\sigma;\tau)\,\mathrm{d}\sigma = \tfrac{1}{12}\,\tau^3\,F''(0;\tau) + \mathcal{O}(\tau^4), \tag{4.3b}$$

with

$$F''(\sigma;\tau) = \mathrm{e}^{\sigma B(\tau)}\,\mathrm{ad}^2_{B(\tau)}(B'(\tau))\,\mathrm{e}^{-\sigma B(\tau)}.$$

Fourth-order modified trapezoidal rule (3.18)**.**

$$Q_4(F,0,\tau) - \int_0^\tau F(\sigma;\tau)\,\mathrm{d}\sigma = \int_0^\tau -\tfrac{1}{24}\,\sigma^2(\tau-\sigma)^2\,F^{(4)}(\sigma;\tau)\,\mathrm{d}\sigma = -\tfrac{1}{720}\,\tau^5\,F^{(4)}(0;t) + \mathcal{O}(\tau^6), \tag{4.3c}$$

with

$$F^{(4)}(\sigma;\tau) = \mathrm{e}^{\sigma B(\tau)}\,\mathrm{ad}^4_{B(\tau)}(B'(\tau))\,\mathrm{e}^{-\sigma B(\tau)}.$$

An analogous representation holds for higher-order Hermite-type quadrature schemes like (3.21).

4.2. The exponential midpoint scheme (2.4)

For the exponential midpoint scheme we now describe the terms influencing the deviation (4.1) in more detail.[9] First we take a closer look at the asymptotic behavior of the defect and the local error itself.

The leading term of the local error $\mathcal{L}(\tau;t_0)$. For $\mathcal{S}(\tau;t_0) = \mathrm{e}^{\tau B(\tau)} = \mathrm{e}^{\tau A(t_0+\frac{\tau}{2})}$, with $\mathcal{S}(0;t_0) = \mathrm{Id}$, the defect is

$$\begin{aligned}\mathcal{D}(\tau;t_0) &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}(\tau;t_0) - A(t_0+\tau)\,\mathcal{S}(\tau;t_0)\\ &= \big(\Gamma(\tau) - A(t_0+\tau)\big)\,\mathcal{S}(\tau;t_0)\\ &= \Big(A(t_0+\tfrac{\tau}{2}) + \int_0^\tau \mathrm{e}^{\sigma A(t_0+\frac{\tau}{2})}\,\tfrac{1}{2}A'(t_0+\tfrac{\tau}{2})\,\mathrm{e}^{-\sigma A(t_0+\frac{\tau}{2})}\,\mathrm{d}\sigma - A(t_0+\tau)\Big)\,\mathcal{S}(\tau;t_0),\end{aligned} \tag{4.4a}$$

satisfying

$$\mathcal{D}(0;t_0) = 0. \tag{4.4b}$$

The derivatives of $\Gamma(\tau)$ at $\tau = 0$ can be derived from the asymptotic expansion (3.10a) in the following way. For the moment, we suppress the argument τ,

$$\Gamma = B + \tau B' + \tfrac{1}{2}\tau^2[B,B'] + \tfrac{1}{6}\tau^3[B,[B,B']] + \mathcal{O}(\tau^4).$$

Thus, straightforward differentiation yields

$$\begin{aligned}\Gamma' = 2\,B'&\\ &+ \tau\big(B'' + [B,B']\big)\\ &+ \tfrac{1}{2}\tau^2\big([B,B''] + [B,[B,B']]\big) + \mathcal{O}(\tau^3).\end{aligned}$$

Furthermore,

$$\begin{aligned}\Gamma'' = 3\,B'' + [B,B']&\\ &+ \tau\big(B''' + 2\,[B,B''] + [B,[B,B']]\big) + \mathcal{O}(\tau^2),\end{aligned}$$

[9] Not all detailed calculations are given here. The results of these calculations have been verified by computer algebra for a general matrix $A(t)$ of dimension 2.

and

$$\Gamma''' = 4\,B''' + 3\,[B, B''] + [B, [B, B']] + \mathcal{O}(\tau).$$

Together with $B^{(m)}(\tau) = 2^{-m} A^{(m)}(t_0 + \frac{\tau}{2})$ this gives

$$\begin{aligned} \Gamma(0) &= A(t_0), \\ \Gamma'(0) &= A'(t_0), \\ \Gamma''(0) &= \tfrac{3}{4} A''(t_0) + \tfrac{1}{2}[A(t_0), A'(t_0)], \\ \Gamma'''(0) &= \tfrac{1}{2} A'''(t_0) + \tfrac{3}{4}[A(t_0), A''(t_0)] + \tfrac{1}{2}[A(t_0), [A(t_0), A'(t_0)]]. \end{aligned} \tag{4.5}$$

We now consider the integral expression (3.4b) for the local error,

$$\mathcal{L}(\tau; t_0) = \int_0^\tau \Pi(\tau, \sigma)\, \mathcal{D}(\sigma; t_0)\, \mathrm{d}\sigma. \tag{4.6}$$

From (4.4a) and (4.6) the fact that, by construction, $\mathcal{D}(\tau; t_0) = \mathcal{O}(\tau^2)$ and $\mathcal{L}(\tau; t_0) = \mathcal{O}(\tau^3)$ is not directly recognizable. A concrete representation is obtained by expanding the defect further; for complexity reasons we will confine ourselves to exactly identifying the asymptotically leading terms. To this end we introduce

$$\mathcal{D}_1(\tau; t_0) = \tfrac{\mathrm{d}}{\mathrm{d}\tau} \mathcal{D}(\tau; t_0) - A(t_0 + \tau)\, \mathcal{D}(\tau; t_0). \tag{4.7a}$$

We temporarily use a simplified notation, where, *e.g.*, (4.4a) is written in the form

$$\mathcal{D} = \mathcal{S}' - A\mathcal{S} = (\Gamma - A)\mathcal{S}.$$

In this notation, and with $\mathcal{S}' = A\,\mathcal{S} + \mathcal{D}$, we obtain

$$\begin{aligned} \mathcal{D}_1 &= \mathcal{D}' - A\mathcal{D} \\ &= \big((\Gamma - A)' + [\Gamma, A]\big)\mathcal{S} + (\Gamma - A)\mathcal{D}, \end{aligned} \tag{4.7b}$$

and

$$\mathcal{D}_1(0; t_0) = \big(\Gamma'(0) - A'(t_0)\big) + [\Gamma(0), A(t_0)] = 0, \tag{4.7c}$$

since $\Gamma(0) = A(t_0)$ and $\Gamma'(0) = A'(t_0)$. Thus, $\mathcal{D}_1(\tau; t_0) = \mathcal{O}(\tau)$.[10]

For

$$\mathcal{D}_2(\tau; t_0) = \tfrac{\mathrm{d}}{\mathrm{d}\tau} \mathcal{D}_1(\tau; t_0) - A(t_0 + \tau)\, \mathcal{D}_1(\tau; t_0), \tag{4.8a}$$

with $\mathcal{S}' = A\,\mathcal{S} + \mathcal{D}$ and $\mathcal{D}' = A\,\mathcal{D} + \mathcal{D}_1$ we obtain

$$\begin{aligned} \mathcal{D}_2 &= \mathcal{D}_1' - A\mathcal{D}_1 \\ &= \big((\Gamma - A)'' + 2\,[\Gamma', A] + [A + \Gamma, A'] + [[\Gamma, A], A]\big)\mathcal{S} \\ &\quad + 2\big((\Gamma - A)' + [\Gamma, A]\big)\mathcal{D} \\ &\quad + (\Gamma - A)\mathcal{D}_1, \end{aligned} \tag{4.8b}$$

and together with (4.4b) and (4.7c),

$$\mathcal{D}_2(0; t_0) = \Gamma''(0) - A''(t_0). \tag{4.8c}$$

Together with (4.5) this gives

$$\mathcal{D}_2(\tau; t_0) = \mathcal{D}_2(0; t_0) + \mathcal{O}(\tau) = \tfrac{1}{2}[A(t_0), A'(t_0)] - \tfrac{1}{4} A''(t_0) + \mathcal{O}(\tau). \tag{4.8d}$$

[10] Of course, this also follows directly from $\mathcal{D}(\tau; t_0) = \mathcal{O}(\tau^2)$.

By integration we finally obtain

$$\begin{aligned}\mathcal{L}(\tau;t_0) &= \int_0^\tau \Pi(\tau,\sigma_1)\,\mathcal{D}(\sigma_1;t_0)\,\mathrm{d}\sigma_1 \\ &= \int_0^\tau \Pi(\tau,\sigma_1)\int_0^{\sigma_1}\Pi(\sigma_1,\sigma_2)\int_0^{\sigma_2}\Pi(\sigma_2,\sigma_3)\,\mathrm{d}\sigma_3\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\mathcal{D}_2(0;t_0)+\mathcal{O}(\tau^4) \\ &=: \underbrace{\mathcal{I}_3(\tau)}_{=\mathcal{O}(\tau^3)}\;\mathcal{D}_2(0;t_0)+\mathcal{O}(\tau^4).\end{aligned}$$

For problems of the type (1.1), with unitary evolution, the triple integral $\mathcal{I}_3(\tau)$ satisfies $\|\mathcal{I}_3(\tau)\|_2 \le \frac{1}{6}\tau^3$, and together with (4.8d) we conclude:

Proposition 4.1. *Consider the solution of* (1.1) *by the exponential midpoint scheme* (2.4)*. If $A \in C^3$, then the local error* (3.1) *satisfies*

$$\|\mathcal{L}(\tau;t_0)\|_2 \le \tfrac{1}{12}\tau^3\big\|[A(t_0),A'(t_0)]-\tfrac{1}{2}A''(t_0)\|_2+\mathcal{O}(\tau^4). \tag{4.9}$$

The leading term of the deviation of the local error estimate. As stated at the beginning of Section 4.1, the deviation $\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)$ consists of two parts.

(i) Asymptotically correct approximation of $\mathcal{L}(\tau;t_0)$ in terms of the exact defect $\mathcal{D}(\tau;t_0)$, see (3.7a): From (4.2) we obtain for $p=2$

$$\tfrac{\tau}{3}\,\mathcal{D}(\tau;t_0)-\mathcal{L}(\tau;t_0)=\int_0^\tau \tfrac{1}{6}\,\sigma(\tau-\sigma)^2\,\tfrac{\mathrm{d}^3}{\mathrm{d}\sigma^3}\big(\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0)\big)\,\mathrm{d}\sigma. \tag{4.10a}$$

Together with

$$\tfrac{\partial}{\partial\sigma}\Pi(\tau,\sigma)=-\Pi(\tau,\sigma)A(t_0+\sigma),$$

we obtain

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\sigma}\big(\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0)\big) &= \Pi(\tau,\sigma)\,\tfrac{\partial}{\partial\sigma}\mathcal{D}(\sigma;t_0)+\tfrac{\partial}{\partial\sigma}\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0) \\ &= \Pi(\tau,\sigma)\big(\tfrac{\partial}{\partial\sigma}\mathcal{D}(\sigma;t_0)-A(t_0+\sigma)\mathcal{D}(\sigma;t_0)\big)=\Pi(\tau,\sigma)\,\mathcal{D}_1(\sigma;t_0),\end{aligned}$$

and

$$\begin{aligned}\tfrac{\mathrm{d}^2}{\mathrm{d}\sigma^2}\big(\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0)\big) &= \tfrac{\mathrm{d}}{\mathrm{d}\sigma}\big(\Pi(\tau,\sigma)\,\mathcal{D}_1(\sigma;t_0)\big) \\ &= \Pi(\tau,\sigma)\big(\tfrac{\partial}{\partial\sigma}\mathcal{D}_1(\sigma;t_0)-A(t_0+\sigma)\mathcal{D}_1(\sigma;t_0)\big)=\Pi(\tau,\sigma)\,\mathcal{D}_2(\sigma;t_0), \\ \tfrac{\mathrm{d}^3}{\mathrm{d}\sigma^3}\big(\Pi(\tau,\sigma)\,\mathcal{D}(\sigma;t_0)\big) &= \tfrac{\mathrm{d}}{\mathrm{d}\sigma}\big(\Pi(\tau,\sigma)\,\mathcal{D}_2(\sigma;t_0)\big) \\ &= \Pi(\tau,\sigma)\big(\tfrac{\partial}{\partial\sigma}\mathcal{D}_2(\sigma;t_0)-A(t_0+\sigma)\mathcal{D}_2(\sigma;t_0)\big)=\Pi(\tau,\sigma)\,\mathcal{D}_3(\sigma;t_0),\end{aligned} \tag{4.10b}$$

with $\mathcal{D}_1$ and $\mathcal{D}_2$ as defined above, and with

$$\mathcal{D}_3(\tau;t_0)=\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{D}_2(\tau;t_0)-A(t_0+\tau)\,\mathcal{D}_2(\tau;t_0). \tag{4.11a}$$

By a straightforward but tedious computation we can obtain

$$\begin{aligned}\mathcal{D}_3 &= \mathcal{D}_2'-A\mathcal{D}_2 \\ &= \big((\Gamma-A)'''+3\,[\Gamma'',A]+[2\,A+\Gamma,A''] \\ &\quad +3\,[\Gamma',A']+[[\Gamma,A],A']+3\,[[\Gamma',A],A]+2\,[[\Gamma,A'],A]+[[A,A'],A]\big)\,\mathcal{S} \\ &\quad +\big(3\,(\Gamma-A)''+6\,[\Gamma',A]+[A+\Gamma,A']+3\,[[\Gamma,A],A]\big)\,\mathcal{D} \\ &\quad +3\big((\Gamma-A)'+[\Gamma,A]\big)\,\mathcal{D}_1 \\ &\quad +(\Gamma-A)\,\mathcal{D}_2,\end{aligned} \tag{4.11b}$$

and together with (4.4b), (4.7c), and (4.8c) we conclude

$$\begin{aligned}\mathcal{D}_3(0;t_0) &= (\Gamma'''(0) - A'''(t_0)) + 3\,[\Gamma''(0), A(t_0)] + [2\,A(t_0) + \Gamma(0), A''(t_0)]\\ &\quad + 3\,[\Gamma'(0), A'(t_0)] + [[\Gamma(0), A(t_0)], A'(t_0)] + 3\,[[\Gamma'(0), A(t_0)], A(t_0)]\\ &\quad + 2\,[[\Gamma(0), A'(t_0)], A(t_0)] + [[A(t_0), A'(t_0)], A(t_0)]\\ &\quad + (\Gamma(0) - A(t_0))(\Gamma''(0) - A''(t_0)).\end{aligned} \tag{4.11c}$$

Together with (4.5) this gives

$$\begin{aligned}\mathcal{D}_3(\tau;t_0) &= \mathcal{D}_3(0;t_0) + \mathcal{O}(\tau)\\ &= -[A(t_0), [A(t_0), A'(t_0)]] + \tfrac{3}{2}[A(t_0), A''(t_0)] - \tfrac{1}{2}\,A'''(t_0) + \mathcal{O}(\tau).\end{aligned} \tag{4.11d}$$

Using $\Pi(\tau,\sigma) = \mathrm{Id} + O(\tau)$, by integration we obtain (see (4.10))

$$\begin{aligned}\tfrac{1}{3}\tau\,\mathcal{D}(\tau;t_0) - \mathcal{L}(\tau;t_0) &= \int_0^\tau \tfrac{1}{6}\,\sigma(\tau-\sigma)^2\,\Pi(\tau,\sigma)\,\mathcal{D}_3(\sigma;t_0)\,\mathrm{d}\sigma = \tfrac{1}{72}\tau^4\mathcal{D}_3(0;t_0) + \mathcal{O}(\tau^5)\\ &= \tau^4\left(-\tfrac{1}{72}[A(t_0),[A(t_0),A'(t_0)]] + \tfrac{1}{48}\tau^4[A(t_0),A''(t_0)] - \tfrac{1}{144}\tau^4\,A'''(t_0)\right) + \mathcal{O}(\tau^5).\end{aligned} \tag{4.12}$$

(ii) Asymptotically correct approximation of $\mathcal{D}(\tau;t_0)$ by $\widetilde{\mathcal{D}}(\tau;t_0)$: We have

$$\widetilde{\mathcal{D}}(\tau;t_0) - \mathcal{D}(\tau;t_0) = \big(\widetilde{\Gamma}(\tau) - \Gamma(\tau)\big)\,\mathcal{S}(\tau;t_0).$$

For the approximate defect $\widetilde{\mathcal{D}}(\tau;t_0)$, version (3.13a), according to (4.3a) with $p=2$,

$$\tfrac{1}{3}\tau\widetilde{\mathcal{D}}(\tau;t_0) - \tfrac{1}{3}\tau\mathcal{D}(\tau;t_0) = \tfrac{1}{36}\tau^4\,[A(t_0),[A(t_0),A'(t_0)]] + \mathcal{O}(\tau^5), \tag{4.13a}$$

where we have used $\mathcal{S}(\tau;t_0) = \mathrm{Id} + \mathcal{O}(\tau)$. For the approximate defect $\widetilde{\mathcal{D}}(\tau;t_0)$, version (3.15), according to (4.3b),

$$\tfrac{1}{3}\tau\,\widetilde{\mathcal{D}}(\tau;t_0) - \tfrac{1}{3}\tau\,\mathcal{D}(\tau;t_0) = \tfrac{1}{72}\tau^4\,[A(t_0),[A(t_0),A'(t_0)]] + \mathcal{O}(\tau^5). \tag{4.13b}$$

Adding (4.12) and (4.13) we finally obtain an estimate for the deviation between the numerical realization of the local error estimate and the true local error:

Proposition 4.2. *Consider the solution of* (1.1) *by the exponential midpoint scheme* (2.4)*. If* $A \in C^4$*, then the deviation* $\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0) = \frac{1}{3}\tau\widetilde{\mathcal{D}}(\tau;t_0) - \mathcal{L}(\tau;t_0)$ *of the local error estimate satisfies*

$$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2 \le \tau^4\big\|c\,[A(t_0),[A(t_0),A'(t_0)]] - \tfrac{1}{48}[A(t_0),A''(t_0)] + \tfrac{1}{144}A'''(t_0)\big\|_2 + \mathcal{O}(\tau^5), \tag{4.14}$$

where $c = \frac{1}{72}$ *for the approximate defect* $\widetilde{\mathcal{D}}(\tau;t_0)$*, version* (3.13a)*, and* $c = 0$ *for the approximate defect* $\widetilde{\mathcal{D}}(\tau;t_0)$*, version* (3.15)*.*

5. Implementation and numerical examples

An algorithmic realization of the fourth-order CFM integrator (2.5) interlaced with the evaluation of the defect-based error estimator (3.7c), (3.16), (3.17), formulated as pseudo-code, is given as follows:

```
ψ = S_1(τ) ψ_0
d = Γ~_1(τ) ψ
d = S_2(τ) d    // (apply 1 additional matrix exponential)
ψ = S_2(τ) ψ   (= ψ_1)
d = d + Γ~_2(τ) ψ − A(t_0 + τ) ψ    // (= approximative defect of ψ_1)
ℓ = τ d/5    // (= local error estimate for ψ_1, scheme of order p = 4)
```

The other versions considered are implemented in a similar fashion.

We now briefly illustrate our theoretical results by computing the empirical orders of the local error and the deviation of the error estimator. To determine the error experimentally, we resort to a reference solution which was computed on a very fine temporal grid.

5.1. Hubbard model

The first test problem we consider is a Hubbard model describing the movement and interaction of electrons within an oxide solar cell [18], with[11] $A(t) \in \mathbb{C}^{400\times 400}$. The explicit time-dependence here originates from an external electric field associated with a photon. Through a Wannier function projection one can map the low energy degrees of freedom onto a set of Wannier orbitals, where each is localized around one vanadium lattice site. Hence, the layers of the solid can be modeled by electrons hopping with amplitude v_{ij} from a Wannier function around site i to one around site j. The Coulomb interaction U between the electrons can be calculated through the constrained random phase approximation, we use $U = 3$.

This model yields the finite-dimensional Hamiltonian

$$H = \frac{1}{2}\sum_{ij\sigma} v_{ij} c^{\dagger}_{j\sigma} c_{i\sigma} + \sum_{ij\sigma\sigma'} U_{ij} \hat{n}_{i\sigma}\hat{n}_{j\sigma'}. \tag{5.1}$$

Here, the 2nd quantization operators $c_{i\sigma}$ and $c^{\dagger}_{j\sigma}$ take an electron away from site i with spin $\sigma \in \{\uparrow,\downarrow\}$ and add it on site j. The occupation number operator $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ tests if there is an electron at site i with spin σ.

The time-dependence in the Hamiltonian (5.1) is introduced through the photon which excites the system out of equilibrium, and which can be described by a classical electric field pulse, see [18]. In our model, we choose $\mathrm{e}^{\mathrm{i}\,\omega(t)}$ with $\omega(t) = \frac{1}{10}\exp\left(-\frac{1}{6}(t-6)^2\cos\left(\frac{7\pi}{4}(t-6)\right)\right)$, which appears in off-diagonal entries of $H(t)$ depending on the geometry underlying the model of the investigated solid.

The Hamiltonian can thus be represented by

$$H(t) = D + f(t)H_S + \mathrm{i}\,g(t)H_A,$$

with a real diagonal matrix D, a real symmetric matrix H_S and a real antisymmetric matrix H_A. The model is described in detail in [21].

The oscillating and quickly attenuating electric field generated by the impact of a photon in this model makes adaptive time-stepping a relevant issue. Thus, the problem can serve to illustrate our theoretical results on local error estimation.

In the following tables, we give the Euclidean norms of the local error $\mathcal{L}(\tau;t_0)$ and of the deviation $\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)$ of defect-based local error estimators $\widetilde{\mathcal{L}}(\tau;t_0)$. As initial state we choose the ground state of the system at $t_0 = 0$.

Tables 2 and 3 give the results for the exponential midpoint scheme, where the evaluation of the integrals appearing in the specification of the error estimator is realized by Taylor quadrature (3.10b) and Hermite-type quadrature (3.14), respectively. As to be expected from the analysis given in Section 4, see Proposition 4.2, the latter variant is more precise by a factor ≈2.

Tables 4 and 5 give the results for the fourth-order CFM integrator (2.5a), where the evaluation of the integrals appearing in the specification of the error estimator is realized by Taylor quadrature (3.10b) ($p = 4$) and the modified Hermite-type quadrature (3.18), respectively.

Tables 6 and 7 give the results for the fourth-order classical Magnus integrator (2.11), where the evaluation of the integrals appearing in the specification of the error estimator is realized by Taylor quadrature (3.10b) ($p = 4$) and the modified Hermite-type quadrature (3.18), respectively.

[11]The dimension of the matrix in this model grows exponentially with the number of considered sites in the Hubbard model of the solid and quickly reaches the limitations of computer hardware, making the issue of an efficient time integrator crucial. For our illustrations in this paper, we choose a manageable model.

TABLE 2. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme applied to (5.1), where Taylor quadrature (3.10b) ($p = 2$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	7.357e−05	2.97	1.794e−05	4.03
3.125e−02	9.120e−06	3.01	1.090e−06	4.04
1.563e−02	1.130e−06	3.01	6.686e−08	4.03
7.813e−03	1.405e−07	3.01	4.135e−09	4.02
3.906e−03	1.750e−08	3.00	2.570e−10	4.01

TABLE 3. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme applied to (5.1), where the trapezoidal quadrature rule (3.14) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	7.357e−05	2.97	3.908e−06	4.13
3.125e−02	9.120e−06	3.01	2.564e−07	3.93
1.563e−02	1.130e−06	3.01	1.666e−08	3.94
7.813e−03	1.405e−07	3.01	1.064e−09	3.97
3.906e−03	1.750e−08	3.00	6.723e−11	3.98

TABLE 4. Local error and deviation of the defect-based error estimator for the fourth order CFM integrator (2.5a) applied to (5.1), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	2.309e−07	5.04	2.619e−08	6.06
3.125e−02	7.146e−09	5.01	3.962e−10	6.05
1.563e−02	2.223e−10	5.01	6.073e−12	6.03
7.813e−03	6.931e−12	5.00	9.324e−14	6.03
3.906e−03	2.164e−13	5.00	1.374e−15	6.08

TABLE 5. Local error and deviation of the defect-based error estimator for the fourth order CFM integrator (2.5a) applied to (5.1), where the modified trapezoidal quadrature rule (3.18) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	2.309e−07	5.04	2.339e−08	6.07
3.125e−02	7.146e−09	5.01	3.544e−10	6.04
1.563e−02	2.223e−10	5.01	5.442e−12	6.03
7.813e−03	6.931e−12	5.00	8.358e−14	6.02
3.906e−03	2.164e−13	5.00	1.249e−15	6.06

TABLE 6. Local error and deviation of the defect-based error estimator for the fourth order classical Magnus integrator (2.11) applied to (5.1), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	1.328e−07	4.67	7.132e−08	6.01
3.125e−02	4.733e−09	4.81	1.073e−09	6.05
1.563e−02	1.569e−10	4.91	1.633e−11	6.04
7.813e−03	5.041e−12	4.96	2.508e−13	6.02
3.906e−03	1.593e−13	4.98	3.699e−15	6.08

TABLE 7. Local error and deviation of the defect-based error estimator for the fourth order classical Magnus integrator (2.11) applied to (5.1), where the modified trapezoidal quadrature rule (3.18) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	Order
6.250e−02	1.328e−07	4.67	1.968e−08	6.11
3.125e−02	4.733e−09	4.81	2.879e−10	6.09
1.563e−02	1.569e−10	4.91	4.323e−12	6.06
7.813e−03	5.041e−12	4.96	6.546e−14	6.05
3.906e−03	1.593e−13	4.98	1.132e−15	5.85

TABLE 8. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme applied to (5.2), where Taylor quadrature (3.10b) ($p = 2$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	Order
1.250e−01	3.343e−03	2.97	4.519e−04	3.97
6.250e−02	4.198e−04	2.99	2.839e−05	3.99
3.125e−02	5.254e−05	3.00	1.777e−06	4.00
1.563e−02	6.569e−06	3.00	1.111e−07	4.00
7.813e−03	8.212e−07	3.00	6.943e−09	4.00

TABLE 9. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme applied to (5.2), where the trapezoidal quadrature rule (3.14) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	Order
1.250e−01	3.343e−03	2.97	5.604e−05	4.11
6.250e−02	4.198e−04	2.99	3.420e−06	4.03
3.125e−02	5.254e−05	3.00	2.124e−07	4.01
1.563e−02	6.569e−06	3.00	1.326e−08	4.00
7.813e−03	8.212e−07	3.00	8.282e−10	4.00

TABLE 10. Local error and deviation of the defect-based error estimator for the fourth order CFM (2.5a) applied to (5.2), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
1.250e−01	1.892e−06	4.99	1.441e−07	5.95
6.250e−02	5.917e−08	5.00	2.271e−09	5.99
3.125e−02	1.850e−09	5.00	3.556e−11	6.00
1.563e−02	5.780e−11	5.00	5.551e−13	6.00
7.813e−03	1.806e−12	5.00	6.530e−15	6.41

TABLE 11. Local error and deviation of the defect-based error estimator for the fourth order CFM (2.5a) applied to (5.2), where the modified trapezoidal quadrature rule (3.18) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
1.250e−01	1.892e−06	4.99	1.184e−07	5.96
6.250e−02	5.917e−08	5.00	1.864e−09	5.99
3.125e−02	1.850e−09	5.00	2.919e−11	6.00
1.563e−02	5.780e−11	5.00	4.556e−13	6.00
7.813e−03	1.806e−12	5.00	6.154e−15	6.21

TABLE 12. Local error and deviation of the defect-based error estimator for the fourth order classical Magnus integrator (2.11) applied to (5.2), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
1.250e-01	5.154e-06	4.97	4.206e-07	5.96
6.250e-02	1.618e-07	4.99	6.612e-09	5.99
3.125e-02	5.064e-09	5.00	1.035e-10	6.00
1.563e-02	1.583e-10	5.00	1.618e-12	6.00
7.813e-03	4.947e-12	5.00	2.109e-14	6.26

TABLE 13. Local error and deviation of the defect-based error estimator for the fourth order classical Magnus integrator (2.11) applied to (5.2), where the modified trapezoidal quadrature rule (3.18) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	Order	$\|\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\|_2$	Order
1.250e−01	5.154e−06	4.97	2.014e−08	6.89
6.250e−02	1.618e−07	4.99	1.817e−10	6.79
3.125e−02	5.064e−09	5.00	1.991e−12	6.51
1.563e−02	1.583e−10	5.00	2.862e−14	6.12
7.813e−03	4.947e−12	5.00	6.848e−15	2.06

5.2. Rosen–Zener model

As a second example, we solve a Rosen-Zener model from [12]. The associated Schrödinger equation in the interaction picture is given by (1.1) with

$$H(t) = f_1(t)\sigma_1 \otimes I_{k\times k} + f_2(t)\sigma_2 \otimes R \in \mathbb{C}^{2k\times 2k}, \quad k = 50, \tag{5.2a}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \tag{5.2b}$$

$$R = \mathrm{tridiag}(1, 0, 1) \in \mathbb{R}^{k\times k}, \tag{5.2c}$$

$$f_1(t) = V_0 \cos(\omega t) \left(\cosh(t/T_0)\right)^{-1}, \qquad f_2(t) = V_0 \sin(\omega t) \left(\cosh(t/T_0)\right)^{-1}, \qquad \omega = \tfrac{1}{2},\ T_0 = 1,\ V_0 = 1\ , \tag{5.2d}$$

subject to the initial condition $\psi(0) = (1, \ldots, 1)^T$.

Tables 8–13 give the results analogous to those for the model (5.1), with the same observations of the empirical convergence orders.

Acknowledgements. This work was supported by the Austrian Science Fund (FWF) under the grant P 30819-N32. We gratefully acknowledge the collaboration with K. Held and A. Kauch (Technische Universität Wien, Institut für Festkörperphysik), who communicated the model of an oxide fuel cell serving as a numerical example.

References

[1] A. Alverman and H. Fehske, High-order commutator-free exponential time-propagation of driven quantum systems. *J. Comput. Phys.* **230** (2011) 5930–5956.

[2] A. Alverman, H. Fehske, and P.B. Littlewood, Numerical time propagation of quantum systems in radiation fields. *New J. Phys.* **14** (2012) 105008.

[3] W. Auzinger, H. Hofstätter, D. Ketcheson and O. Koch, Practical splitting methods for the adaptive integration of nonlinear evolution equations. Part I: Construction of optimized schemes and pairs of schemes. *BIT* **57** (2017) 55–74.

[4] W. Auzinger, O. Koch and M. Thalhammer, Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part II: Higher-order methods for linear problems. *J. Comput. Appl. Math.* **255** (2013) 384–403.

[5] W. Auzinger, O. Koch and M. Thalhammer, Defect-based local error estimators for high-order splitting methods involving three linear operators. *Numer. Algorithms* **70** (2015) 61–91.

[6] P. Bader, A. Iserles, K. Kropielnicka and P. Singh, Effective approximation for the linear time-dependent Schrödinger equation. *Found. Comput. Math.* **14** (2014) 689–720.

[7] P. Bader, A. Iserles, K. Kropielnicka and P. Singh, Efficient methods for linear Schrödinger equation in the semiclassical regime with time-dependent potential. *Proc. R. Soc. A* **472** (2016) 20150733.

[8] W. Bao and Y. Cai, Mathematical theory and numerical methods for Bose–Einstein condensation. *Kinet. Relat. Mod.* **6** (2013) 1–135.

[9] S. Blanes, F. Casas, A. Farrés, J. Laskar, J. Makazaga and A. Murua, New families of symplectic splitting methods for numerical integration in dynamical astronomy. *Appl. Numer. Math.* **68** (2013) 58–72.

[10] S. Blanes, F. Casas, J.A. Oteo and J. Ros, The Magnus expansion and some of its applications. *Phys. Rep.* 470 (2008) 151–238.

[11] S. Blanes, F. Casas and J. Ros, Improved high order integrators based on the Magnus expansion. *BIT* **40** (2000) 434–450.

[12] S. Blanes, F. Casas and M. Thalhammer, High-order commutator-free quasi–Magnus integrators for non-autonomous linear evolution equations. *Comput. Phys. Commun.* **220** (2017) 243–262.

[13] S. Blanes and P.C. Moan, Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems. *Appl. Numer. Math.* **56** (2005) 1519–1537.

[14] Y. Cao and L. Petzold, A posteriori error estimate and global error control for ordinary differential equations by the adjoint method. *SIAM J. Sci. Comput.* **26** (2004) 359–374.

[15] E. Celledoni, A. Iserles, S.P. Nørsett and B. Orel, Complexity theory for Lie-group solvers. *J. Complexity* **18** (2002) 242–286.

[16] E. Hairer, Ch. Lubich and G. Wanner, Geometric Numerical Integration. 2nd edition. Springer-Verlag, Berlin–Heidelberg–New York (2006).

[17] E. Hairer, S.P. Nørsett and G. Wanner, Solving Ordinary Differential Equations I. Springer-Verlag, Berlin–Heidelberg–New York (1987).

[18] K. Held, Electronic structure calculations using dynamical mean field theory. *Adv. Phys.* **56** (2007) 829–926.

[19] N. Higham, Functions of Matrices. Theory and Computations. SIAM, Philadelphia, PA (2008).

[20] M. Hochbruck and C. Lubich, On Magnus integrators for time-dependent Schrödinger equations. *SIAM J. Numer. Anal.* **41** (2003) 945–963.

[21] M. Innerberger, *Modeling of solar cells by small Hubbard clusters.* B.Sc. thesis, Vienna University of Technology (2017).

[22] A. Iserles, K. Kropielnicka and P. Singh, Magnus–Lanczos methods with simplified commutators for the Schrödinger equation with a time-dependent potential. *SIAM J. Numer. Anal.* **56** (2018) 1547–1569.

[23] A. Iserles and S.P. Nørsett, On the solution of linear differential equations on Lie groups. *Phil. Trans. R. Soc. Lond. A* **357** (1999) 983–1019.

[24] K. Kormann, S. Holmgren and H.O. Karlsson, Accurate time-propagation of the Schrödinger equation with an explicitly time-dependent Hamiltonian. *J. Chem. Phys.* **128** (2008) 184101.

[25] K. Kormann, S. Holmgren and H.O. Karlsson, Global error control of the time-propagation for the Schrödinger equation with a time-dependent Hamiltonian. *J. Comput. Sci.* **2** (2011) 178–187.

[26] C. Lubich, From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis. *Zurich Lectures in Advanced Mathematics*. European Mathematical Society, Zurich (2008).

[27] W. Magnus, On the exponential solution of differential equations for a linear operator. *Comm. Pure Appl. Math.* **7** (1954) 649–673.

[28] M. Thalhammer, A fourth-order commutator-free exponential integrator for nonautonomous differential equations. *SIAM J. Numer. Anal.* **44** (2012) 851–864.