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A POSTERIORI ERROR ESTIMATION FOR MAGNUS-TYPE INTEGRATORS *

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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 a model of solar cells composed of heterostructures based on transition metal oxides.

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1. INTRODUCTION AND OVERVIEW

Problem. We study systems of linear ordinary differential equations

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

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 [26] 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

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For $A(t)$ of the form (1.1), the evolution operator $\mathcal{E}(\tau; t_0)$ is unitary. It can be (formally) represented by the Magnus series (2.7) [25].

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)* [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]. In [11] the algebraic framework underlying a systematic construction is discussed. Yet another interesting approach was applied to the Schrödinger equation in [7, 8], 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 [19]. This leads to the derivation of so-called commutator-free Magnus-type integrators in [8].
Alternative approaches to the construction of favorable integrators based on the evaluation of exponentials rely on the Magnus expansion. The seminal references to the classical Magnus approach are [20,24], 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. 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]. 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.
An a priori theoretical error analysis for Magnus integrators of second and fourth order has first been given in [18] 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 [26], where order reductions are observed, however.

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 [5, 6]. A posteriori error estimation and adaptive step selection for Magnus-type integrators is to our knowledge only discussed in [22], where classical Magnus integrators are endowed with a global error estimator based on integration of an adjoint problem as suggested in [14].
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 [10]. This allows to employ efficient high-order adaptive splitting methods proposed and analyzed for instance in [4, 6]. For these, a large body of theory has been developed in recent years, see for instance [9,15,23] and references therein. In [21], 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 practical merits of our adaptive approach relying on defect-based error estimators, also as compared to adaptive splitting methods, will be assessed in the forthcoming study [3].
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.

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 [24]: The solution to a time-dependent system (1.1) can be represented by

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

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

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

with the Bernoulli numbers b_k.
Numerical integrators can be obtained by truncating the Magnus expansion (2.7b) and a suitable approximation $\Omega(\tau)$ to the arising multi-dimensional integral representation for $\boldsymbol{\Omega}(\tau)$ by numerical quadrature, and defining ψ_1 by (2.1) with

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

A detailed exposition on this approach is given for example in [11] and in [15].
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, 8, 12].

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 $c = (c_1, \ldots, c_K) \in [0, 1]^K$.

(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

$$\begin{gathered} c = \Big(\tfrac{1}{2} - \tfrac{\sqrt{15}}{10}\,, \tfrac{1}{2}, \tfrac{1}{2} + \tfrac{\sqrt{15}}{10}\Big)\,, \\ B_1(\tau) = \tau A_2(\tau)\,, \quad B_2(\tau) = \tfrac{\sqrt{15}}{3}\,\tau\big(A_3(\tau) - A_1(\tau)\big)\,, \quad B_3(\tau) = \tfrac{10}{3}\tau\big(A_1(\tau) - 2\,A_2(\tau) + A_3(\tau)\big), \\ C_1(\tau) = \big[B_1(\tau), B_2(\tau)\big], \quad C_2(\tau) = -\tfrac{1}{60}\big[B_1(\tau), 2\,B_3(\tau) + C_1(\tau)\big], \\ \Omega(\tau) = B_1(\tau) + \tfrac{1}{12}\,B_3(\tau) + \tfrac{1}{240}\big[-20\,B_1(\tau) - B_3(\tau) + C_1(\tau), B_2(\tau) + C_2(\tau)\big]\,, \end{gathered} \tag{2.12}$$

see [11, Eq. (251)].

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 [5,6].

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

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

and hence,

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

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

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

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

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

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 $\tfrac{\mathrm{d}^{p+1}}{\mathrm{d}\sigma^{p+1}}\,\widehat{\mathcal{D}}(\sigma;t_0)$. 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 $\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathcal{S}(\tau;t_0)$ 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

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

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 Sec. 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 $\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\Omega(\tau)}$, 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

Fréchet 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 [15, Sec. III.4, (4.3)]. This implies that the Fréchet derivative of

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

takes the form

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

see [15, Sec. III.4, Lemma 1].
An alternative representation even more useful for our purpose is given by the integral formula (see [17, Sec. 10.2, (10.15)])

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

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[1]

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

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

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

A computable approximation for the time derivative $\tfrac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{e}^{\tau B(\tau)}$ 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

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

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

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

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

Here one may apply conventional interpolatory quadrature or, as a better choice, 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 $\mathrm{ad}^m_{B(\tau)}(B'(\tau))$. 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 $T_p(F,0,\tau)$.
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,

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

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 $j=1,2$,

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

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

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

Then, (3.16) takes the form

$$\begin{aligned}\widetilde{\mathcal{D}}(\tau;t_0) &= \big(B_2(\tau) + C_2^+(\tau) - A(t_0+\tau)\big)\,\mathcal{S}(\tau;t_0)\\ &\quad + \mathcal{S}_2(\tau)\big(B_1(\tau) + C_1^+(\tau) + C_2^-(\tau)\big)\,\mathcal{S}_1(\tau) + \mathcal{S}(\tau;t_0)\,C_1^-(\tau)\,.\end{aligned} \tag{3.20}$$

This requires the evaluation of three 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 quadrature

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

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

$$\begin{aligned}B'(\tau) &= \tfrac{1}{2}\big(c_1A'(t_0+c_1\tau) + c_2A'(t_0+c_2\tau)\big)\\ &\quad - \tfrac{\sqrt{3}}{12}\,[A(t_0+c_1\tau), A(t_0+c_2\tau)]\\ &\quad - \tfrac{\sqrt{3}}{12}\,\tau\big(c_1\,[A'(t_0+c_1\tau), A(t_0+c_2\tau)] + c_2\,[A(t_0+c_1\tau), A'(t_0+c_2\tau)]\big)\,.\end{aligned}$$

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),

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

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

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

Then, (3.22) takes the form

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

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

	CFM-type estimator			Classical 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)	$k=1$	3	(3.25)	$k=1$	1

TABLE 1. Additional computational effort for error estimators.

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). In the following, we give a more precise characterization of the error of the error estimate, i.e., of the deviation

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

4.1. Classification of terms influencing the deviation (4.1)

Two different asymptotically correct approximations are involved in the construction of the local error estimate $\widetilde{\mathcal{L}}(\tau;t_0) = \frac{1}{p+1}\tau\widetilde{\mathcal{D}}(\tau;t_0) \approx \mathcal{L}(\tau;t_0)$ (see (3.7)):

(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 associated defect $\mathcal{D}(\tau;t_0)$ by a computable object $\widetilde{\mathcal{D}}(\tau;t_0)$ via quadrature, see (3.7b) and Sec. 3.3, and 3.4.

The approximation errors can be characterized as follows:

ad (i): The approximation (3.7a) admits another interpretation, namely as an Hermite-type quadrature for the local error integral (3.4b), involving only a single evaluation[2] of the defect $\mathcal{D}(\tau;t_0)$ (cf. [5,6]). 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

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

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

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

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).

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

4.2. **The exponential midpoint scheme** (2.4)

In the following, we confine ourselves to the case of the exponential midpoint scheme, $p = 2$, which represents both a commutator-free and a classical Magnus integrator, and describe the terms influencing the deviation (4.1) in more detail.[3] 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

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

Furthermore,

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

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,

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

[3]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.

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, $\mathcal{D}_1(\tau;t_0) = \mathcal{O}(\tau)$.[4]
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

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

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

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

Together with (4.5) this gives

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

By integration we finally obtain

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

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

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

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*

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

The leading term of the deviation of the local error estimate. As stated at the beginning of Sec. 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

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

By integration we obtain (see (4.10))

$$\tfrac{1}{3}\tau\,\mathcal{D}(\tau;t_0) - \mathcal{L}(\tau;t_0) = \int_0^\tau \tfrac{1}{6}\,\sigma(\tau-\sigma)^2\,\Pi(\tau,\sigma)\,\mathcal{D}_3(\sigma;t_0)\,\mathrm{d}\sigma = \mathcal{O}(\tau^4)\,,$$

For problems of the type (1.1), with unitary evolution, this gives

$$\|\tfrac{\tau}{3}\,\mathcal{D}(\tau;t_0) - \mathcal{L}(\tau;t_0)\| \le \tfrac{1}{72}\tau^4\,\|\mathcal{D}_3(0;t_0)\| + \mathcal{O}(\tau^5)\,, \tag{4.12}$$

with $\mathcal{D}_3(0;t_0)$ from (4.11d).

(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 $p=2$,

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

For the approximate defect $\widetilde{\mathcal{D}}(\tau;t_0)$, version (3.15), according to (4.3b),

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

Combining (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* $\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0) = \tfrac{1}{3}\tau\widetilde{\mathcal{D}}(\tau;t_0) - \mathcal{L}(\tau;t_0)$ *of the local error estimate satisfies*

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

where $c = \frac{1}{24}$ *for the approximate defect* $\widetilde{\mathcal{D}}(\tau;t_0)$, *version* (3.13a), *and* $c = \frac{1}{36}$ *for the approximate defect* $\widetilde{\mathcal{D}}(\tau;t_0)$, *version* (3.15).

5. Implementation and numerical example

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 = Γ̃_1(τ) ψ
d = S_2(τ) d    // (apply 1 additional matrix exponential)
ψ = S_2(τ) ψ    (= ψ_1)
d = d + Γ̃_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.
The test problem we consider is a Hubbard model describing the movement and interaction of electrons within an oxide solar cell [16], with $A(t) \in \mathbb{C}^{400\times 400}$. The explicit time-dependence here originates from an external electric field associated with a photon. The Hamiltonian can 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 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 Euclidian 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 quadrature (3.14), respectively. As to be expected from the analysis given in Sec. 4, see Proposition 4.2, the latter variant is more precise by a factor ≈ 2.

τ	$\Vert\mathcal{L}(\tau;t_0)\Vert_2$	p	$\Vert\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\Vert_2$	p
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 2. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme, where Taylor quadrature (3.10b) ($p = 2$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\Vert\mathcal{L}(\tau;t_0)\Vert_2$	p	$\Vert\widetilde{\mathcal{L}}(\tau;t_0) - \mathcal{L}(\tau;t_0)\Vert_2$	p
1.250e−01	5.759e−04	2.71	6.859e−05	4.69
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 3. Local error and deviation of the defect-based error estimator for the exponential midpoint scheme, where the trapezoidal quadrature rule (3.14) is used for the evaluation of $\widetilde{\mathcal{D}}$.

Tables 4 and 5 give the results for the fourth-order CFM-type 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 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 quadrature (3.18), respectively.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	p	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	p
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 4. Local error and deviation of the defect-based error estimator for (2.5a), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	p	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	p
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 5. Local error and deviation of the defect-based error estimator for (2.5a), where the modified trapezoidal quadrature rule (3.18) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	p	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	p
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 6. Local error and deviation of the defect-based error estimator for (2.11), where Taylor quadrature (3.10b) ($p = 4$) is used for the evaluation of $\widetilde{\mathcal{D}}$.

τ	$\|\mathcal{L}(\tau;t_0)\|_2$	p	$\|\widetilde{\mathcal{L}}(\tau;t_0)-\mathcal{L}(\tau;t_0)\|_2$	p
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 7. Local error and deviation of the defect-based error estimator for (2.11), where the trapezoidal quadrature rule (3.14) is used for the evaluation of $\widetilde{\mathcal{D}}$.

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