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A FOURTH-ORDER COMMUTATOR-FREE EXPONENTIAL INTEGRATOR FOR NONAUTONOMOUS DIFFERENTIAL EQUATIONS*

MECHTHILD THALHAMMER†

Abstract. In the present work, we study the convergence behavior of commutator-free exponential integrators for abstract nonautonomous evolution equations

$$u'(t) = A(t)u(t), \qquad 0 < t \leq T.$$

In particular, we focus on a fourth-order scheme that relies on the composition of two exponentials involving the values of the linear operator family A at the Gaussian nodes

$$u_1 = \mathrm{e}^{h(a_2 A_1 + a_1 A_2)}\, \mathrm{e}^{h(a_1 A_1 + a_2 A_2)}\, u_0, \quad a_i = \tfrac{1}{4} \pm \tfrac{\sqrt{3}}{6}\,, \quad c_i = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}\,, \quad A_i = A(c_i h), \quad i = 1, 2.$$

We prove that the numerical scheme is stable and derive an error estimate with respect to the norm of the underlying Banach space. The theoretically expected order reduction is illustrated by a numerical example for a parabolic initial-boundary value problem subject to a homogeneous Dirichlet boundary condition.

Key words. exponential integrators, commutator-free methods, nonautonomous differential equations, parabolic evolution equations, stability, convergence

AMS subject classifications. 65L05, 65M12, 65J10

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1. Introduction.

In the present paper, we consider a nonautonomous differential equation involving a time-dependent linear operator A

$$u'(t) = A(t)u(t), \quad 0 < t \leq T, \qquad u(0) \text{ given.} \tag{1.1}$$

Our setting includes parabolic initial-boundary value problems that take the form (1.1) when written as an abstract initial value problem on a Banach space. The objective of this work is to analyze the error behavior of the fourth-order commutator-free exponential integrator

$$\begin{gathered} u_1 = \mathrm{e}^{h(a_2 A_1 + a_1 A_2)}\, \mathrm{e}^{h(a_1 A_1 + a_2 A_2)}\, u_0, \\ a_i = \tfrac{1}{4} \pm \tfrac{\sqrt{3}}{6}, \quad c_i = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}, \quad A_i = A(c_i h), \qquad i = 1, 2, \end{gathered} \tag{1.2}$$

to explain the substantial order reduction for problems of parabolic type. For that purpose, we derive a representation for the defect of (1.2) which remains valid within the framework of sectorial operators and analytic semigroups. In situations where $A(t)$ is a bounded linear operator, the Campbell–Baker–Hausdorff formula is a powerful tool for the error analysis of (1.2) and higher-order schemes, respectively. However, it is problematic to justify its validity in the context of parabolic evolution equations.

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†Institut für Mathematik, Universität Innsbruck, Technikerstrasse 13, 6020 Innsbruck, Austria (Mechthild.Thalhammer@uibk.ac.at).

Therefore, in this paper, we follow a different approach based on the variation-of-constants formula.

Numerical schemes that involve the evaluation of the exponential and related functions were proposed in the middle of the past century; for a historical review, see [24]. At present, a variety of works confirms the renewed interest in such exponential integrators; as a small selection, we mention the recent works [5, 8, 14, 16, 19, 20] and refer to the references given therein. A reason for these research activities are advances in the computation of the product of a matrix exponential with a vector; see, for instance, [10, 15, 25]. As a consequence, numerical integrators based on the Magnus expansion [23] and related method classes [2, 3, 6, 7, 17, 21] are practicable in the numerical solution of nonautonomous stiff differential equations; see also [11, 12, 30] and references cited therein.

The excellent error behavior of interpolatory Magnus integrators for time-dependent Schrödinger equations is explained in Hochbruck and Lubich [14]. There, it is proved that the exponential midpoint rule applied to ordinary differential equations (1.1)

$$u_1 = \mathrm{e}^{hA_1}\, u_0, \qquad A_1 = A\big(\tfrac{h}{2}\big), \tag{1.3}$$

is convergent of order 2 without any restriction on the size of $h\big\|A(t)\big\|$. Moreover, under a mild stepsize restriction, a fourth-order error bound is valid for the Magnus integrator

$$u_1 = \mathrm{e}^{ha_1(A_1+A_2)+h^2a_2[A_2,A_1]}\, u_0,$$
$$a_1 = \tfrac{1}{2}, \quad a_2 = \tfrac{\sqrt{3}}{12}, \quad c_i = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}, \quad A_i = A(c_ih), \qquad i = 1,2,$$

where $\big[A_1, A_2\big] = A_1A_2 - A_2A_1$ denotes the matrix commutator. In [11], we considered the numerical scheme (1.3) in the context of parabolic evolution equations and showed that the full convergence order 2 is obtained when the error is measured in the norm of the underlying Banach space, provided that the data and the exact solution of (1.1) are sufficiently smooth in time.

The purpose of the present work is to investigate the convergence properties of higher-order methods for linear nonautonomous parabolic problems (1.1). Provided that the time-dependent sectorial operator $A(t)$ is Hölder-continuous with respect to t, it is ensured that any linear operator defined through $B = \alpha A(\xi_1) + (1-\alpha)A(\xi_2)$ with $\alpha, \xi_1, \xi_2 \in \mathbb{R}$ generates an analytic semigroup $\big(\mathrm{e}^{tB}\big)_{t\geq 0}$, that is, numerical schemes such as (1.2) remain well defined for abstract evolution equations (1.1). For that reason, we focus on commutator-free exponential integrators that rely on the composition of exponentials involving linear combinations of values of A. We show that the fourth-order scheme (1.2) is stable; however, unless the operator familiy A fulfills unnatural requirements, a substantial order reduction is encountered. For instance, for one-dimensional initial-boundary value problems subject to a homogeneous Dirichlet boundary condition, the order of convergence with respect to a discrete L^p-norm is $2 + \kappa$, where $0 \leq \kappa < (2p)^{-1}$, in general.

The present work is organized as follows. In section 2, we first state the fundamental hypotheses on the nonautonomous evolution equation (1.1). The considered commutator-free exponential integration scheme is then introduced in section 3. The numerical approximation is based on the composition of two exponentials that involve the values of A at certain nodal points. Sections 4 and 5 are concerned with a stability and convergence analysis for parabolic problems. In section 5.1, we derive an expansion of the numerical solution defect which remains well defined for abstract differential equations (1.1) involving an unbounded linear operator $A(t)$, provided that the data and the exact solution of the problem are sufficiently many times differentiable with respect to time. The main result, a convergence estimate for the fourth-order scheme (1.2), is given in section 5.2. Important tools for its proof are the stability bound and the representation of the defect derived before. Section 6 is devoted to a numerical example that illustrates the expected order reduction.

2. Parabolic problems. Henceforth, we denote by $(X, \|\cdot\|_X)$ the underlying Banach space. Our basic requirements on the unbounded linear operator family A defining the right-hand side of the differential equation in (1.1) are that of [11, 30]. For a detailed treatise of time-dependent evolution equations we refer to [22, 29]. The monographs [13, 27] delve into the theory of sectorial operators and analytic semigroups.

HYPOTHESIS 1. *We assume that the densly defined and closed linear operator $A(t) : D \subset X \to X$ is uniformly sectorial for $0 \le t \le T$. Thus, there exist constants $a \in \mathbb{R}$, $0 < \phi < \frac{\pi}{2}$, and $M > 0$ such that for all $0 \le t \le T$ the resolvent of $A(t)$ satisfies the condition*

$$\Big\| \big(\lambda I - A(t)\big)^{-1} \Big\|_{X \leftarrow X} \le \frac{M}{|\lambda - a|} \tag{2.1}$$

for any complex number $\lambda \notin S_\phi(a) = \big\{\lambda \in \mathbb{C} : |\arg(a-\lambda)| \le \phi\big\} \cup \{a\}$. The graph norm of $A(t)$ and the norm in D fulfill the following relation with a constant $K > 0$:

$$K^{-1}\|x\|_D \le \|x\|_X + \big\|A(t)x\big\|_X \le K\|x\|_D, \qquad x \in D, \qquad 0 \le t \le T.$$

Moreover, it holds $A \in \mathscr{C}^\vartheta\big([0,T], L(D,X)\big)$ for some $0 < \vartheta \le 1$, i.e., the bound

$$\big\|A(t) - A(s)\big\|_{X \leftarrow D} \le L(t-s)^\vartheta, \qquad 0 \le s \le t \le T, \tag{2.2}$$

is valid with a constant $L > 0$.

For any $0 \le s \le T$ the sectorial operator $\Omega = A(s)$ generates an analytic semigroup $\big(\mathrm{e}^{t\Omega}\big)_{t \ge 0}$ on X which is defined by means of the integral formula of Cauchy

$$\mathrm{e}^{t\Omega} = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \mathrm{e}^\lambda \big(\lambda I - t\Omega\big)^{-1} \,\mathrm{d}\lambda, \quad t > 0, \qquad \mathrm{e}^{t\Omega} = I, \quad t = 0. \tag{2.3}$$

Here, Γ denotes a path that surrounds the spectrum of Ω.

Henceforth, for $0 < \mu < 1$, we denote by X_μ some intermediate space between the Banach spaces $D = X_1$ and $X = X_0$ such that the norm in X_μ satisfies the bound $\|x\|_{X_\mu} \le K\|x\|_D^\mu \|x\|_X^{1-\mu}$ with a constant $K > 0$ for all elements $x \in D$. Examples for intermediate spaces are real interpolation spaces (see Lunardi [22]) or fractional power spaces (see Henry [13]). Then, for all $0 \le \mu \le \nu \le 1$ and integers $k \ge 0$ the following bound is valid:

$$\big\|t^{k+\nu-\mu}\,\Omega^k\,\mathrm{e}^{t\Omega}\big\|_{X_\nu \leftarrow X_\mu} \le M, \qquad 0 \le t \le T, \tag{2.4}$$

with a constant $M > 0$. As a consequence, the linear operator φ_m which is given by

$$\varphi_m(t\Omega) = \frac{1}{(m-1)!\,t^m} \int_0^t \mathrm{e}^{(t-\tau)\Omega}\,\tau^{m-1}\mathrm{d}\tau, \quad t > 0, \qquad \varphi_m(0) = \frac{1}{(m-1)!}\,I, \tag{2.5a}$$

for integers $m \geq 1$, remains bounded on X_μ for any $0 \leq t \leq T$ and $0 \leq \mu \leq 1$. In the subsequent sections, we make use of the identities

$$\text{(2.5b)} \qquad \mathrm{e}^{t\Omega} = I + t\Omega\,\varphi_1(t\Omega), \qquad \varphi_{m-1}(t\Omega) = \frac{1}{(m-1)!}\,I + t\Omega\,\varphi_m(t\Omega), \quad m \geq 1.$$

Furthermore, it is substantial that the relation

$$\text{(2.5c)} \qquad \varphi_m(t\Omega) - \varphi_m(0) = t\Omega\,\chi(t\Omega)$$

holds with a linear operator $\chi(t\Omega)$ that is bounded on X_μ; see [13, 22] and also [11, 30].

3. Commutator-free exponential integrator. In this section, we introduce an integration method for linear nonautonomous parabolic problems (1.1) which relies on the composition of two exponentials. We note that the considered scheme is an example of a *Crouch–Grossman method* [9].

For a constant stepsize $h > 0$ the associated grid points are denoted by $t_j = jh$ for $j \geq 0$. The numerical approximation $u_{n+1} \approx u(t_{n+1})$ to the true solution of (1.1) is given by the recurrence formula

$$\text{(3.1a)} \qquad u_{n+1} = \mathrm{e}^{\widetilde{\zeta}hC_n}\,\mathrm{e}^{\zeta hB_n}\,u_n, \qquad n \geq 0.$$

Here, we employ the following abbreviations:

$$\text{(3.1b)} \qquad \begin{aligned} A_{ni} &= A(t_n + c_i h), \qquad i = 1, 2, \\ B_n = \alpha A_{n1} + \beta A_{n2}, &\qquad C_n = \gamma A_{n1} + \delta A_{n2}. \end{aligned}$$

Throughout, we assume that the nodal points $\zeta, \widetilde{\zeta}, c_1, c_2 \in \mathbb{R}$ and the coefficients $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ satisfy

$$\text{(3.1c)} \quad 0 < \zeta < 1, \qquad \widetilde{\zeta} = 1 - \zeta, \qquad 0 \leq c_1 \leq c_2 \leq 1, \qquad \alpha + \beta = 1, \qquad \gamma + \delta = 1.$$

The following remark shows that relation (3.1a) remains well defined within the analytical framework of section 2.

Remark 1. Under the assumptions of Hypothesis 1, the linear operator

$$\alpha A_{n1} + (1-\alpha)A_{n2} = A_{n2} + \alpha\big(A_{n1} - A_{n2}\big), \qquad \alpha \in \mathbb{R},$$

is sectorial; see also [13, Theorem 1.3.2]. Therefore, the commutator-free exponential integrator (3.1) is well defined for abstract evolution equations (1.1).

4. Stability. The stability properties of the commutator-free exponential integrator (3.1) are determined by the behavior of the evolution operator

$$\text{(4.1)} \qquad \prod_{i=m}^{n} \mathrm{e}^{\widetilde{\zeta}hC_i}\,\mathrm{e}^{\zeta hB_i} = \mathrm{e}^{\widetilde{\zeta}hC_n}\,\mathrm{e}^{\zeta hB_n}\,\mathrm{e}^{\widetilde{\zeta}hC_{n-1}}\,\mathrm{e}^{\zeta hB_{n-1}} \cdots \mathrm{e}^{\widetilde{\zeta}hC_m}\,\mathrm{e}^{\zeta hB_m},$$

where $n \geq m \geq 0$. The following result implies that the numerical solution u_n remains bounded for arbitrarily chosen stepsizes $h > 0$ as long as $nh \leq T$.

THEOREM 1 (stability). *Under the requirements of Hypothesis* 1 *on A, the discrete evolution operator* (4.1) *fulfills the bound*

$$\Big\| \prod_{i=m}^{n} \mathrm{e}^{\widetilde{\zeta}hC_i}\,\mathrm{e}^{\zeta hB_i} \Big\|_{X \leftarrow X} \leq M, \qquad 0 \leq mh \leq nh \leq T,$$

with a constant $M > 0$ that does not depend on n and h.

Proof. As in our preceeding works [11, 30], the proof of the above stability result relies on the telescopic identity and the integral formula of Cauchy. In the present situation, it is useful to compare the discrete evolution operator (4.1) with the linear operator

$$\prod_{i=m}^{n} \mathrm{e}^{\widetilde{\zeta} h A_{m2}}\, \mathrm{e}^{\zeta h A_{m2}} = \prod_{i=m}^{n} \mathrm{e}^{h A_{m2}} = \mathrm{e}^{(t_{n+1}-t_m) A_{m2}},$$

which satisfies the well-known bound

$$\left\| \mathrm{e}^{(t_{n+1}-t_m)A_{m2}} \right\|_{X\leftarrow X} + \left\| (t_{n+1}-t_m)\, A_{m2}\, \mathrm{e}^{(t_{n+1}-t_m)A_{m2}} \right\|_{X\leftarrow X} \leq C$$

for $0 \leq t_m \leq t_n \leq T$. Therefore, it suffices to estimate the difference

$$\begin{aligned}
\Delta_m^n &= \prod_{i=m}^{n} \mathrm{e}^{\widetilde{\zeta} h C_i}\, \mathrm{e}^{\zeta h B_i} - \mathrm{e}^{(t_{n+1}-t_m)A_{m2}} \\
&= \sum_{j=m}^{n-1} \Delta_{j+1}^n \Big(\mathrm{e}^{\widetilde{\zeta} h C_j}\, \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} \Big) \mathrm{e}^{(t_j - t_m)A_{m2}} \\
&\quad + \sum_{j=m}^{n} \mathrm{e}^{(t_{n+1}-t_{j+1})A_{m2}} \Big(\mathrm{e}^{\widetilde{\zeta} h C_j}\, \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} \Big) \mathrm{e}^{(t_j - t_m)A_{m2}}.
\end{aligned}$$

For this purpose, it is notable that the following relation holds true:

$$\mathrm{e}^{\widetilde{\zeta} h C_j} \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} = \Big(\mathrm{e}^{\widetilde{\zeta} h C_j} - \mathrm{e}^{\widetilde{\zeta} h A_{m2}} \Big) \mathrm{e}^{\zeta h B_j} + \mathrm{e}^{\widetilde{\zeta} h A_{m2}} \Big(\mathrm{e}^{\zeta h B_j} - \mathrm{e}^{\zeta h A_{m2}} \Big).$$

By means of the integral formula of Cauchy, the resolvent identity

$$(\lambda I - \Omega_1)^{-1} - (\lambda I - \Omega_2)^{-1} = (\lambda I - \Omega_1)^{-1} (\Omega_1 - \Omega_2) (\lambda I - \Omega_2)^{-1},$$

and the relations given in (3.1), we receive

$$\begin{aligned}
&\Big(\mathrm{e}^{\widetilde{\zeta} h C_j}\, \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} \Big)\, \mathrm{e}^{(t_j - t_m)A_{m2}} \\
&\quad = \frac{\widetilde{\zeta} h}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^{\lambda}\, (\lambda - \widetilde{\zeta} h C_j)^{-1} \big(\gamma (A_{j1} - A_{j2}) + A_{j2} - A_{m2} \big) \\
&\qquad\qquad \times (\lambda - \widetilde{\zeta} h A_{m2})^{-1}\, \mathrm{e}^{\zeta h B_j}\, \mathrm{e}^{(t_j - t_m)A_{m2}}\, \mathrm{d}\lambda \\
&\qquad + \frac{\zeta h}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^{\lambda}\, \mathrm{e}^{\widetilde{\zeta} h A_{m2}}\, (\lambda - \zeta h B_j)^{-1} \big(\alpha (A_{j1} - A_{j2}) + A_{j2} - A_{m2} \big) \\
&\qquad\qquad \times (\lambda - \zeta h A_{m2})^{-1}\, \mathrm{e}^{(t_j - t_m)A_{m2}}\, \mathrm{d}\lambda.
\end{aligned}$$

With the help of the resolvent bound (2.1), the Hölder estimate (2.2) for A, and (2.4) it thus follows

$$\begin{aligned}
\left\| \Big(\mathrm{e}^{\widetilde{\zeta} h C_j}\, \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} \Big)\, \mathrm{e}^{(t_j - t_m)A_{m2}} \right\|_{X\leftarrow X} &\leq M h^{\vartheta}, \qquad j = m, \\
\left\| \Big(\mathrm{e}^{\widetilde{\zeta} h C_j}\, \mathrm{e}^{\zeta h B_j} - \mathrm{e}^{h A_{m2}} \Big)\, \mathrm{e}^{(t_j - t_m)A_{m2}} \right\|_{X\leftarrow X} &\leq M h (t_j - t_m)^{-1+\vartheta}, \qquad j > m.
\end{aligned}$$

Consequently, a further application of (2.4) together with a Gronwall-type inequality with a weakly singular kernel (see also [4, 26]) yields the desired stability bound. ∎

5. Convergence. In this section, we analyze the convergence behavior of the considered commutator-free exponential integrator for parabolic problems (1.1). As a first step, we next derive a useful relation for the defect of (3.1) by means of a suitable linearization of the differential equation and an application of the variation-of-constants formula. Similar techniques have been used in the study of exponential splitting methods; see [1, 18, 28] and references therein. The following considerations also explain the definition of the numerical method.

5.1. Expansion of the defect. Replacing in (3.1) the numerical by the exact solution values defines the defect of the method

$$u(t_{n+1}) = \mathrm{e}^{\widetilde{\zeta} h C_n}\, \mathrm{e}^{\zeta h B_n}\, u(t_n) + d_{n+1}, \qquad n \geq 0. \tag{5.1}$$

Our basic approach is to consider the initial value problem (1.1) on the subinterval $[t_n, t_{n+1}]$ and to derive an analogous relation to (3.1a) for the exact solution values. For that purpose, we set

$$G_n(t) = \big(A(t) - B_n\big)u(t), \qquad H_n(t) = \big(A(t) - C_n\big)u(t). \tag{5.2}$$

On the one hand, rewriting the right-hand side of the differential equation in (1.1) as $u'(t) = B_n u(t) + G_n(t)$ and applying the variation-of-constants formula (see [22]) yields the following relation for the solution value at time $t_n + \zeta h$:

$$u(t_n + \zeta h) = \mathrm{e}^{\zeta h B_n}\, u(t_n) + \int_0^{\zeta h} \mathrm{e}^{(\zeta h - \tau) B_n}\, G_n(t_n + \tau)\, \mathrm{d}\tau.$$

On the other hand, by linearizing (1.1) around C_n and inserting the above representation for $u(t_n + \zeta h)$, we further obtain

$$\begin{aligned} u(t_{n+1}) = \mathrm{e}^{\widetilde{\zeta} h C_n}\, \mathrm{e}^{\zeta h B_n}\, u(t_n) + \mathrm{e}^{\widetilde{\zeta} h C_n} \int_0^{\zeta h} \mathrm{e}^{(\zeta h - \tau) B_n}\, G_n(t_n + \tau)\, \mathrm{d}\tau \\ + \int_0^{\widetilde{\zeta} h} \mathrm{e}^{(\widetilde{\zeta} h - \tau) C_n}\, H_n(t_n + \zeta h + \tau)\, \mathrm{d}\tau. \end{aligned}$$

Consequently, the defect of the numerical method (3.1) equals

$$d_{n+1} = \mathrm{e}^{\widetilde{\zeta} h C_n} \int_0^{\zeta h} \mathrm{e}^{(\zeta h - \tau) B_n}\, G_n(t_n + \tau)\, \mathrm{d}\tau + \int_0^{\widetilde{\zeta} h} \mathrm{e}^{(\widetilde{\zeta} h - \tau) C_n}\, H_n(t_n + \zeta h + \tau)\, \mathrm{d}\tau. \tag{5.3}$$

In order to derive a suitable expansion of d_{n+1}, it is useful to introduce some additional notation.

The time derivatives of the linear operator A and the exact solution u of (1.1) at time t_n are denoted by

$$A_n^{(i)} = A^{(i)}(t_n), \quad i \geq 0, \qquad \widehat{u}_n^{(j)} = u^{(j)}(t_n), \quad j \geq 0. \tag{5.4a}$$

For the coefficients of the numerical scheme, we define

$$\mu_i = \alpha c_1^i + \beta c_2^i, \qquad \nu_i = \gamma c_1^i + \delta c_2^i, \qquad i = 1, 2, 3; \tag{5.4b}$$

see (3.1). We note that for a sufficiently differentiable function $f : [t_n, t_{n+1}] \to X$ a Taylor series expansion yields

$$\begin{aligned} f(t_n + \tau) &= \sum_{i=0}^{m} \frac{\tau^i}{i!} f_n^{(i)} + R\big(\tau^{m+1}, f^{(m+1)}\big), \qquad 0 \le \tau \le h, \\ R\big(\tau^{m+1}, f^{(m+1)}\big) &= \frac{1}{m!} \tau^{m+1} \int_0^1 (1-\sigma)^m f^{(m+1)}(t_n + \sigma\tau)\, \mathrm{d}\sigma, \end{aligned} \tag{5.5}$$

where $f_n^{(i)} = f^{(i)}(t_n)$. Thus, provided that the quantity

$$\big\| f^{(m+1)} \big\|_{X,\infty} = \max_{t_n \le t \le t_{n+1}} \big\| f^{(m+1)}(t) \big\|_X$$

is well defined, the remainder fulfills

$$\big\| R\big(\tau^{m+1}, f^{(m+1)}\big) \big\|_X \le M h^{m+1} \big\| f^{(m+1)} \big\|_{X,\infty}, \qquad 0 \le \tau \le h,$$

with some constant $M > 0$. Terms that satisfy an estimate of this form are henceforth denoted by $\mathscr{R}\big(h^{m+1}, f^{(m+1)}\big)$. In particular, the abbreviation $\mathscr{R}\big(h^k, A^{(i)}\, u^{(j)}\big)$ signifies that the bound

$$\big\| \mathscr{R}\big(h^k, A^{(i)}\, u^{(j)}\big) \big\|_X \le M h^k \max_{t_n \le s,t \le t_{n+1}} \big\| A^{(i)}(s)\, u^{(j)}(t) \big\|_{X,\infty}$$

holds true.

Provided that the involved derivatives of A and u are well defined, the following representation is valid for the defect d_{n+1} given by (5.1). We recall formula (2.5a) for the linear operator φ_m.

LEMMA 1. *The numerical solution defect of* (3.1) *fulfills the relation*

$$\begin{aligned} d_{n+1} = \sum_{(i,j) \in \mathscr{J}} & h^{i+j+1}\, \Phi_{ij}\, A_n^{(i)} \widehat{u}_n^{(j)} + \mathscr{R}\big(h^5, A^{(4)} u\big) \\ & + \mathscr{R}\big(h^5, A''' u'\big) + \mathscr{R}\big(h^5, A'' u''\big) + \mathscr{R}\big(h^5, A' u'''\big), \end{aligned}$$

where $\Phi_{ij} = \Phi_{ij}(hB_n, hC_n)$ *is defined through*

$$\begin{aligned} \Phi_{ij} = \frac{1}{i!j!} \bigg\{ & \zeta^{j+1} \mathrm{e}^{\widetilde{\zeta} h C_n} \Big((i+j)!\, \zeta^i \varphi_{i+j+1}(\zeta h B_n) - j!\, \mu_i \varphi_{j+1}(\zeta h B_n) \Big) \\ & + \sum_{\ell=j+1}^{i+j} \ell!\, \tbinom{i+j}{\ell} \zeta^{i+j-\ell} \widetilde{\zeta}^{\ell+1} \varphi_{\ell+1}(\widetilde{\zeta} h C_n) \\ & + \sum_{\ell=0}^{j} \ell!\, \zeta^{j-\ell} \widetilde{\zeta}^{\ell+1} \Big(\tbinom{i+j}{\ell} \zeta^i - \nu_i \tbinom{j}{\ell} \Big) \varphi_{\ell+1}(\widetilde{\zeta} h C_n) \bigg\} \end{aligned}$$

and $\mathscr{J} = \big\{(1,0), (2,0), (1,1), (3,0), (2,1), (1,2)\big\}$.

Proof. We first derive a useful relation for the maps G_n and H_n defined in (5.2). With the help of (5.5), by combining the expansions

$$\begin{aligned} A(t_n + \tau) - B_n &= \sum_{i=0}^{3} \frac{1}{i!} \big(\tau^i - \mu_i h^i\big) A_n^{(i)} + \mathscr{R}\big(h^4, A^{(4)}\big), \\ u(t_n + \tau) &= \sum_{j=0}^{2} \frac{1}{j!} \tau^j \widehat{u}_n^{(j)} + R\big(\tau^3, u^{(3)}\big), \end{aligned}$$

we receive the following representation:

$$
\begin{aligned}
G_n(t_n+\tau) &= \sum_{(i,j)\in\mathscr{J}} \frac{1}{i!j!}\big(\tau^i-\mu_i h^i\big)\tau^j A_n^{(i)}\widehat{u}_n^{(j)} + \mathscr{R}\big(h^4\big),\\
\mathscr{R}\big(h^4\big) &= \mathscr{R}\big(h^4,A^{(4)}u\big)+\mathscr{R}\big(h^4,A'''u'\big)+\mathscr{R}\big(h^4,A''u''\big)+\mathscr{R}\big(h^4,A'u'''\big);
\end{aligned} \tag{5.6a}
$$

see also (3.1b)–(3.1c) and (5.4). Similarly, it follows

$$
H_n(t_n+\zeta h+\tau) = \sum_{(i,j)\in\mathscr{J}} \frac{1}{i!j!}\big((\zeta h+\tau)^i-\nu_i h^i\big)(\zeta h+\tau)^j A_n^{(i)}\widehat{u}_n^{(j)} + \mathscr{R}\big(h^4\big). \tag{5.6b}
$$

We next insert the above expansions (5.6) into (5.3) and express the resulting integrals by means of (2.5a). Altogether, this yields the given result. ◻

In the situation of Section 2, a reasonable smoothness assumption on (1.1) is that the linear operator A and the exact solution u are sufficiently differentiable with respect to the variable t. Precisely, we suppose $A^{(4)}(t)$ and $u^{(4)}(t)$ to be bounded in the underlying Banach space X for all $0\le t\le T$. The following remark states that then the expansion of Lemma 1 is well-defined. However, unless the exact solution satisfies additional (unnatural) requirements such as $A'(t)u(t)\in D$ for $0\le t\le T$, in general, it is not possible to further expand the defect.

Remark 2. Provided that $u'(t)\in X$ it follows from the differential equation in (1.1) that $A(t)u(t)\in X$ and therefore $u(t)\in D$ for $0\le t\le T$. Differentiating (1.1) with respect to the variable t implies $A(t)u'(t)=u''(t)-A'(t)u(t)\in X$, and, as a consequence, $u'(t)\in D$ for any $0\le t\le T$. Similarly, it follows $u^{(j-1)}(t)\in D$ if $u^{(j)}(t)\in X$ for $0\le t\le T$ and $j=3,4$. Thus, under the regularity requirements $A\in\mathscr{C}^4\big([0,T],L(D,X)\big)$ and $u\in\mathscr{C}^4\big([0,T],X\big)$, the representation of the defect given in Lemma 1 is well defined.

5.2. Error estimate. With the help of the stability estimate and the expansion of the defect given in sections 4 and 5.1, we are able to prove the following convergence result.

THEOREM 2 (convergence). *Assume that the requirements of Hypothesis* 1 *are fulfilled and that further* $A\in\mathscr{C}^4\big([0,T],L(D,X)\big)$ *and* $u\in\mathscr{C}^4\big([0,T],X\big)$. *Then, provided that* $A^{(i)}(t)\,u^{(j)}(t)$ *belongs to the intermediate space* X_κ *with* $0\le\kappa<1$ *for* $0\le t\le T$ *and* $(i,j)\in\big\{(1,0),(2,0),(1,1)\big\}$, *the fourth-order commutator-free exponential integrator* (1.2) *satisfies the error estimate*

$$
\|u_n-u(t_n)\|_X \le C\Big(\big\|u_0-u(0)\big\|_X + h^{2+\kappa}\big(1+|\log h|\big)\Big), \qquad 0\le t_n\le T,
$$

with some constant $C>0$ *independent of* n *and* h.

Proof. In order to obtain a suitable relation for the global error $e_n=u_n-u(t_n)$, we first resolve the recurrence formula (3.1a) for the numerical approximation

$$
u_n=\prod_{i=0}^{n-1}\mathrm{e}^{\widetilde{\zeta}hC_i}\,\mathrm{e}^{\zeta hB_i}\,u_0, \qquad n\ge 0.
$$

Furthermore, by using (5.1), we receive $e_n=e_n^{(1)}+e_n^{(2)}$ with

$$
e_n^{(1)}=\prod_{i=0}^{n-1}\mathrm{e}^{\widetilde{\zeta}hC_i}\,\mathrm{e}^{\zeta hB_i}\big(u_0-u(0)\big), \qquad e_n^{(2)}=-\sum_{j=0}^{n-1}\prod_{i=j+1}^{n-1}\mathrm{e}^{\widetilde{\zeta}hC_i}\,\mathrm{e}^{\zeta hB_i}\,d_{j+1}. \tag{5.7}
$$

We next estimate the terms in (5.7) with respect to the norm of the underlying Banach space X. An application of Theorem 1 shows that the first term is bounded by a constant times the error of the initial value

$$\big\|e_n^{(1)}\big\|_X \leq \Bigg\|\prod_{i=0}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\Bigg\|_{X\leftarrow X} \|u_0 - u(0)\|_X \leq C\|u_0-u(0)\|_X.$$

For estimating the second term $e_n^{(2)}$, we employ the representation of the defect given in Lemma 1. Making use of the fact that the sums involving the remainder and the terms where $i+j\geq 3$ are bounded by constant times h^3, we receive

$$\begin{aligned}
\big\|e_n^{(2)}\big\|_X \leq h^2 \sum_{j=0}^{n-1} &\Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{10}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} \big\|A_j'\widehat{u}_j\big\|_{X_\kappa}\\
&+ h^3 \sum_{j=0}^{n-1} \Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{20}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} \big\|A_j''\widehat{u}_j\big\|_{X_\kappa}\\
&+ h^3 \sum_{j=0}^{n-1} \Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{11}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} \big\|A_j'\widehat{u}_j'\big\|_{X_\kappa}\\
&+ Ch^3.
\end{aligned} \tag{5.8}$$

We note that the coefficients of the fourth-order scheme (1.2) satisfy the conditions

$$\begin{aligned}
\Phi_{20}(0,0) &= \tfrac12\Big\{\zeta\big(\tfrac13\,\zeta^2-\mu_2\big)+\widetilde{\zeta}\Big(\tfrac13\,\widetilde{\zeta}^2+\zeta\widetilde{\zeta}+\zeta^2-\nu_2\Big)\Big\}=0,\\
\Phi_{11}(0,0) &= \zeta^2\big(\tfrac13\,\zeta-\tfrac12\,\mu_1\big)+\widetilde{\zeta}\Big(\tfrac13\,\widetilde{\zeta}^2+\tfrac12\,\widetilde{\zeta}(2\zeta-\nu_1)+\zeta(\zeta-\nu_1)\Big)=0.
\end{aligned} \tag{5.9a}$$

Therefore, similar arguments as in the proof of Theorem 1 show the refined bounds

$$\begin{aligned}
\Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{20}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} &\leq Mh(t_n-t_j)^{-1+\kappa},\\
\Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{11}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} &\leq Mh(t_n-t_j)^{-1+\kappa};
\end{aligned}$$

see also (2.4) and (2.5c). In relation (5.8), it remains to estimate the sum involving Φ_{10}. For that purpose, we apply (2.5b) together with suitable Taylor expansions of B_j and C_j. Moreover, the coefficients of (1.2) fulfill

$$\begin{aligned}
\Phi_{10}(0,0) &= \zeta\big(\tfrac12\,\zeta-\mu_1\big)+\tfrac12\,\widetilde{\zeta}^2+\widetilde{\zeta}(\zeta-\nu_1)=0,\\
\Psi_{10}(0,0) &= \zeta^2\big(\tfrac16\,\zeta-\tfrac12\,\mu_1\big)+\widetilde{\zeta}\Big(\tfrac16\,\widetilde{\zeta}^2+\tfrac12\,\widetilde{\zeta}(\zeta-\nu_1)+\zeta\big(\tfrac12\,\zeta-\mu_1\big)\Big)=0.
\end{aligned} \tag{5.9b}$$

As a consequence, we finally obtain the refined estimate

$$\Bigg\|\prod_{i=j+1}^{n-1} \mathrm{e}^{\widetilde{\zeta} hC_i}\,\mathrm{e}^{\zeta hB_i}\,\Phi_{10}(hB_j,hC_j)\Bigg\|_{X\leftarrow X_\kappa} \leq Mh^{1+\kappa}\big(1+|\log h|+(t_{n+1}-t_m)^{-1}\big).$$

Altogether, this implies

$$\begin{aligned}\big\|e_n^{(2)}\big\|_X &\le Ch^{3+\kappa}\sum_{j=0}^{n-1}\big(1+|\log h|+(t_n-t_j)^{-1}\big)\\ &\quad + Ch^4\sum_{j=0}^{n-1}(t_n-t_j)^{-1+\kappa}+Ch^3 \le Ch^{2+\kappa}\big(1+|\log h|\big),\end{aligned}$$

which proves the given error estimate. □

Remark 3. Going over the proof of Theorem 2 shows that the essential conditions for a fractional convergence order of $2+\kappa$ are (5.9). We note that the conditions for a classical convergence order 3 are equivalent to the relations in (5.9). However, it is not possible to construct a commutator-free exponential integrator of classical order 3 that is based on the evaluation of one exponential only, that is, the validity of relation (5.9) implies $0<\zeta<1$ in (3.1).

6. Numerical example.

In this section, we illustrate the error estimate of Theorem 2 by a numerical example for a parabolic initial boundary value problem subject to a homogeneous Dirichlet boundary condition. We start with a brief discussion of the considered time integration schemes. For notational simplicity, we give only the first step and denote $A_i = A(c_i h)$.

Method 1. For parabolic problems (1.1), it follows from the error estimate given in our previous work [11] that the exponential midpoint rule

$$u_1 = \mathrm{e}^{hA_1}\, u_0, \qquad c_1 = \tfrac{1}{2},$$

is convergent of order 2 with respect to the norm of the underlying Banach space.

Method 2. The commutator-free exponential integration scheme

$$\begin{gathered} u_1 = \mathrm{e}^{(1-\zeta)h(a_1A_1+(1-a_1)A_2)}\,\mathrm{e}^{\zeta h A_1}\, u_0,\\ \zeta = \tfrac{\sqrt{3}}{3}\,, \qquad a_1 = \tfrac{1}{4}-\tfrac{\sqrt{3}}{4}\,, \qquad c_i = \tfrac{1}{2}\mp\tfrac{\sqrt{3}}{6}\,, \qquad i=1,2,\end{gathered}$$

has a classical convergence order 3.

Method 3. The numerical method

$$u_1 = \mathrm{e}^{h(a_2A_1+a_1A_2)}\,\mathrm{e}^{h(a_1A_1+a_2A_2)}\, u_0, \qquad a_i = \tfrac{1}{4}\pm\tfrac{\sqrt{3}}{6}\,, \qquad c_i = \tfrac{1}{2}\mp\tfrac{\sqrt{3}}{6}\,, \qquad i=1,2,$$

is the unique scheme of the form (3.1) that satisfies the conditions for a classical convergence order 4; see also (1.2).

In the numerical example, as an illustration, the fourth-order commutator-free exponential integrator given before is compared with a fourth-order interpolatory Magnus integrator. To explain the stability and error behavior of this method for parabolic problems is beyond the purpose of the present work.

Method 4. The fourth-order interpolatory Magnus integrator

$$u_1 = \mathrm{e}^{ha_1(A_1+A_2)+h^2a_2[A_2,A_1]}\, u_0, \qquad a_1 = \tfrac{1}{2}\,, \qquad a_2 = \tfrac{\sqrt{3}}{12}\,,$$

requires the evaluation of the linear operator $\big[A_2, A_1\big] = A_2A_1 - A_1A_2$.

TABLE 6.1
Numerical temporal convergence orders in a discrete L^1-norm for spatial discretizations of grid length $\Delta x = (M+1)^{-1}$.

Stepsize h	1/2	1/4	1/8	1/16	1/32
Method 1 (M = 50)	2.0076	1.9632	1.9597	1.9699	1.9822
Method 1 (M = 100)	2.0075	1.9631	1.9595	1.9696	1.9818
Method 2 (M = 50)	1.0924	1.9634	2.2295	2.3162	2.4248
Method 2 (M = 100)	1.0949	1.9604	2.2267	2.3153	2.4181
Method 3 (M = 50)	2.2597	2.1983	2.3386	2.4337	2.4999
Method 3 (M = 100)	2.2591	2.1960	2.3348	2.4227	2.4782
Method 4 (M = 50)	3.3250	3.5115	3.3419	3.0490	2.8486
Method 4 (M = 100)	3.0426	3.4011	3.4838	3.2384	2.9488

TABLE 6.2
Numerical temporal convergence orders in a discrete L^2-norm for spatial discretizations of grid length $\Delta x = (M+1)^{-1}$.

Stepsize h	1/2	1/4	1/8	1/16	1/32
Method 1 (M = 50)	2.0120	1.9740	1.9723	1.9786	1.9879
Method 1 (M = 100)	2.0120	1.9739	1.9722	1.9785	1.9878
Method 2 (M = 50)	1.1979	1.9223	2.0992	2.1336	2.1732
Method 2 (M = 100)	1.1985	1.9208	2.0977	2.1303	2.1666
Method 3 (M = 50)	2.0197	2.0409	2.1271	2.1917	2.2331
Method 3 (M = 100)	2.0194	2.0397	2.1244	2.1859	2.2210
Method 4 (M = 50)	3.3204	3.5217	2.9654	2.4024	2.3609
Method 4 (M = 100)	3.0341	3.4204	3.3656	2.6010	2.3197

We consider a one-dimensional initial boundary value problem for a real-valued function $U : [0,1] \times [0,T] \to \mathbb{R} : (x,t) \mapsto U(x,t)$ comprising the partial differential equation

$$\partial_t U(x,t) = \mathscr{A}(x,t)\, U(x,t), \qquad 0 < x < 1, \quad 0 < t \le T, \tag{6.1a}$$

subject to a homogeneous Dirichlet boundary condition and an initial condition

$$U(0,t) = 0 = U(1,t), \quad 0 \le t \le T, \qquad U(x,0) = U_0(x), \quad 0 \le x \le 1. \tag{6.1b}$$

The differential equation involves a second-order differential operator

$$\mathscr{A}(x,t) = \alpha(x,t)\, \partial_x^2 + \beta(x,t)\, \partial_x + \gamma(x,t) \tag{6.1c}$$

which we assume to satisfy the condition of strong ellipticity. We further suppose that the space and time-dependent coefficients α, β, and γ fulfill suitable regularity and boundedness requirements. For $v \in \mathscr{C}_0^\infty(0,1)$ we define $u(t)$ and $A(t)$ through $\big(u(t)\big)(x) = U(x,t)$ and $\big(A(t)v\big)(x) = \mathscr{A}(x,t)v(x)$. Then, problem (6.1) can be cast into the abstract framework of section 2 for

$$X = L^p(0,1), \qquad D = W^{p,2}(0,1) \cap W_0^{p,1}(0,1), \qquad 1 < p < \infty;$$

see [11] and references therein. In view of the numerical experiment, we choose

$$\alpha(x,t) = \mathrm{e}^{x-t}, \qquad \beta(x,t) = xt, \qquad \gamma(x,t) = x^2\big(1 + \mathrm{e}^t\big).$$

The admissible values of κ in Theorem 2 are $0 \le \kappa < (2p)^{-1}$. Thus, the expected fractional convergence order in $X = L^p(0,1)$ is $2 + \kappa$, where $\kappa < (2p)^{-1}$.

Table 6.3
Numerical temporal convergence orders in a discrete L^∞-norm for spatial discretizations of grid length $\Delta x = (M+1)^{-1}$.

Stepsize h	1/2	1/4	1/8	1/16	1/32
Method 1 (M = 50)	2.0250	2.0065	2.0208	2.0226	2.0149
Method 1 (M = 100)	2.0250	2.0063	2.0207	2.0222	2.0129
Method 2 (M = 50)	1.2328	1.7318	1.8169	1.8604	1.9092
Method 2 (M = 100)	1.2341	1.7313	1.8135	1.8559	1.9072
Method 3 (M = 50)	1.7384	1.8369	1.9113	1.9649	1.9851
Method 3 (M = 100)	1.7391	1.8347	1.9103	1.9604	1.9736
Method 4 (M = 50)	3.3042	3.0169	1.9200	2.0864	2.1880
Method 4 (M = 100)	3.0257	3.4434	2.0132	1.9839	2.0752

In the numerical experiment, we discretize the problem in space by symmetric finite differences of grid length $\Delta x = (M+1)^{-1}$. In time, we apply the exponential integrators given above with stepsize $h = 2^{-i}$ for $1 \leq i \leq 5$ and integrate the problem up to time $T = 1$. A reference solution is determined for a temporal stepsize $h = 2^{-10}$. The numerical temporal order of convergence with respect to a discrete L^p-norm is determined in a standard way from the numerical solution values. The obtained numbers for $p = 2$ and the limiting cases $p = 1$ and $p = \infty$ are displayed in Tables 6.1, 6.2, and 6.3. The convergence order 2 for the exponential midpoint rule (Method 1) is explained by a convergence result proved in [11]. For the commutator-free exponential integrators of classical order 3 (Method 2) and classical order 4 (Method 3), respectively, the values of approximately $2 + (2p)^{-1}$ are in accordance with the convergence orders predicted by Theorem 2.

7. Conclusions. In the present work, we studied the convergence properties of a commutator-free exponential integrator that relies on the composition of two exponentials for parabolic initial value problems of the form (1.1). In particular, we focused on the fourth-order scheme (1.2), which is based on the Gaussian nodes. We showed that the exponential integration scheme remains stable for arbitrarily large stepsizes. But, it is seen from the theoretical investigations and as well in a numerical experiment that a substantial order reduction occurs, in general. For instance, for one-dimensional parabolic initial-boundary value problems under a homogeneous Dirichlet boundary condition a fractional convergence order of at most $2+(2p)^{-1}$ can be expected in the norm of the function space L^p. The order reduction is explained by the fact that even if the exact solution of the initial boundary value problem belongs to the domain of the differential operator and further is temporally smooth, it in general does not fulfill additional boundary conditions, that is, combinations of the form $A(s)A(t)u(t)$ are not well defined for all $0 \leq s, t \leq T$.

For that reason, concerning the derivation of high-order exponential integrators for nonautonomous parabolic problems, it seems more promising to employ a suitable linearization and to base the numerical schemes on explicit exponential methods of Runge–Kutta or multistep type. Also, the error analysis for nonautonomous parabolic equations is of theoretical value as it gives insight into how to construct and study numerical methods for quasi-linear equations which are of particular interest in view of practical applications. For example, quasi-linear parabolic problems are used in the modeling of diffusion processes with state-dependent diffusivity and arise in the study of fluids in porous media, see [12]. We intend to investigate this approach in a future work.

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