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A second-order Magnus-type integrator for nonautonomous parabolic problems

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Abstract

We analyse stability and convergence properties of a second-order Magnus-type integrator for linear parabolic differential equations with time-dependent coefficients, working in an analytic framework of sectorial operators in Banach spaces. Under reasonable smoothness assumptions on the data and the exact solution, we prove a second-order convergence result without unnatural restrictions on the time stepsize. However, if the error is measured in the domain of the differential operator, an order reduction occurs, in general. A numerical example illustrates and confirms our theoretical results.

Keywords: Linear parabolic problems; Time-dependent coefficients; Magnus integrators; Exponential integrators; Stability; Convergence

1. Introduction

In this paper, we are concerned with the numerical solution of nonautonomous linear differential equations

$$u'(t) = A(t)u(t) + b(t), \quad 0 < t \leqslant T, \quad u(0) = u_0. \tag{1}$$

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In particular, we are interested in analysing the situation where (1) constitutes an abstract parabolic problem on a Banach space. The precise assumptions on the operator family $A(t)$, $0\leqslant t\leqslant T$, are given in Section 2.

For linear matrix differential equations $y'(t)=A(t)y(t)$ with possibly noncommuting matrices $A(t)$, Magnus [11] has constructed the solution in the form $y(t)=\exp(\Omega(t))y(0)$ with a matrix $\Omega(t)$ depending on iterated integrals of $A(t)$, see also [5, Section IV.7]. Only recently, this Magnus expansion has been exploited numerically by approximating the arising integrals by quadrature methods, see [9,16] within the context of geometric integration and [1] in connection with the time-dependent Schrödinger equation.

As the convergence of the Magnus expansion is only guaranteed if $\|\Omega(t)\|<\pi$, stiff problems with large or even unbounded $\|A(t)\|$ seemed to be excluded. However, in an impressing paper [8], Hochbruck and Lubich give error bounds for Magnus integrators applied to time-dependent Schrödinger equations, solely working with matrix commutator bounds. The aim of the present paper is to derive the corresponding result for a second-order Magnus-type integrator applied to linear parabolic differential equations with time-dependent coefficients, exploiting the temporal regularity of the exact solution. For that purpose, we employ an abstract formulation of the partial differential equation and work within the framework of sectorial operators and analytic semigroups in Banach spaces.

The paper is organised as follows. In Section 2, we state the main assumptions on the problem and its numerical discretisation. Our numerical scheme for (1) is a mixed method that integrates the homogeneous part by a second-order Magnus integrator and the inhomogeneity by the exponential midpoint rule. In Section 3, we first study the stability properties of the Magnus integrator. The given stability bounds form the basis for the convergence results specified in Section 4. Under the main assumption that the data and the exact solution are sufficiently smooth in time, the actual order of convergence depends on the chosen norm in which the error is measured as well as on the boundary values of a certain function, depending itself on the data of the problem. For instance, for a second-order strongly elliptic differential operator with smooth coefficients, we obtain second-order convergence with respect to the L^p-norm for $1<p<\infty$. However, if the error is measured in the domain of the differential operator, an order reduction down to $1+1/(2p)$ is encountered, in general. These theoretical results are illustrated and confirmed by a numerical experiment given in Section 5.

Throughout the paper, $C>0$ denotes a generic constant.

2. Equation and numerical method

In the sequel, we introduce the basic assumptions on (1) and specify the numerical scheme. For a detailed treatise of time-dependent evolution equations we refer to [10,15]. The monographs [6,14] delve into the theory of sectorial operators and analytic semigroups.

We first consider abstract initial value problems of the form (1) with $b=0$. Our fundamental requirement on the map A defining the right-hand side of the equation is the following.

Hypothesis 1. Let $(X,\|\cdot\|_X)$ and $(D,\|\cdot\|_D)$ be Banach spaces with D densely embedded in X. We suppose that the closed linear operator $A(t)\colon D\to X$ is uniformly sectorial for $0\leqslant t\leqslant T$. Thus, there exist constants $a\in\mathbb{R}$, $0<\phi<\pi/2$, and $M_1\geqslant 1$ such that $A(t)$ satisfies the following resolvent condition on the complement of the sector $S_\phi(a) = \{\lambda \in \mathbb{C} : |\arg(a-\lambda)| \leqslant \phi\} \cup \{a\}$

$$\|(\lambda I - A(t))^{-1}\|_{X \leftarrow X} \leqslant \frac{M_1}{|\lambda - a|} \quad \text{for any } \lambda \in \mathbb{C} \backslash S_\phi(a). \tag{2}$$

Besides, we assume that the graph norm of $A(t)$ and the norm in D are equivalent, i.e., for every $0 \leqslant t \leqslant T$ and for all $x \in D$ the estimate

$$C_v^{-1} \|x\|_D \leqslant \|x\|_X + \|A(t)x\|_X \leqslant C_v \|x\|_D \tag{3}$$

holds with some constant $C_v \geqslant 1$.

We remark that for any linear operator $F : X \to D$ relation (3) implies

$$\|A(t)F\|_{X \leftarrow X} \leqslant C_v \|F\|_{D \leftarrow X} \quad \text{and} \quad \|F\|_{D \leftarrow X} \leqslant C_v (1 + \|A(t)F\|_{X \leftarrow X}). \tag{4}$$

As a consequence, for fixed $0 \leqslant s \leqslant T$, the sectorial operator $A(s)$ generates an analytic semigroup $(\mathrm{e}^{tA(s)})_{t \geqslant 0}$ which satisfies the bound

$$\|\mathrm{e}^{tA(s)}\|_{X \leftarrow X} + \|\mathrm{e}^{tA(s)}\|_{D \leftarrow D} + \|t\mathrm{e}^{tA(s)}\|_{D \leftarrow X} \leqslant M_2 \quad \text{for } 0 \leqslant t \leqslant T \tag{5}$$

with some constant $M_2 \geqslant 1$, see e.g., [10].

In view of our convergence and stability results it is essential that $A(t)$ is Hölder-continuous with respect to t.

Hypothesis 2. We assume $A \in C^\alpha([0, T], L(D, X))$ for some $0 < \alpha \leqslant 1$, i.e., the following estimate is valid with a constant $M_3 > 0$

$$\|A(t) - A(s)\|_{X \leftarrow D} \leqslant M_3 (t - s)^\alpha \tag{6}$$

for all $0 \leqslant s \leqslant t \leqslant T$.

The nonautonomous problem (1) with $b = 0$ is discretised by a Magnus integrator which is of classical order 2. For this, let $t_j = jh$ be the grid points associated with a constant stepsize $h > 0$, $j \geqslant 0$. Then, for some initial value $u_0 \in X$, the numerical approximation u_{n+1} to the true solution at time t_{n+1} is defined recursively by

$$u_{n+1} = \mathrm{e}^{hA_n} u_n, \quad n \geqslant 0 \quad \text{where } A_n = A\left(t_n + \frac{h}{2}\right). \tag{7}$$

This method was studied for time-dependent Schrödinger equations in [8].

We next extend (7) to initial value problems (1) with an additional inhomogeneity $b : [0, T] \to X$. Motivated by the time-invariant case, we approximate the inhomogeneity by the exponential midpoint rule. This yields the recursion

$$u_{n+1} = \mathrm{e}^{hA_n} u_n + h\varphi(hA_n) b_n, \quad n \geqslant 0 \quad \text{with } b_n = b\left(t_n + \frac{h}{2}\right), \tag{8}$$

where the linear operator $\varphi(hA_n)$ is given by

$$\varphi(hA_n) = \frac{1}{h} \int_0^h \mathrm{e}^{(h-\tau)A_n} \, \mathrm{d}\tau. \tag{9}$$

The competitiveness of the numerical scheme (8) relies on an efficient calculation of the exponential and the related function (9). More precisely, the product of a matrix exponential and a vector has to be computed. It has been shown in [2,7] that Krylov methods prove to be excellent for this aim.

We note for later use that the estimates (4) and (5) imply

$$\|\varphi(hA_n)\|_{X\leftarrow X} + \|\varphi(hA_n)\|_{D\leftarrow D} + \|h\varphi(hA_n)\|_{D\leftarrow X} \leqslant M_4 \tag{10}$$

with some constant $M_4 \geqslant 1$.

In the following example we show that linear parabolic problems with time-dependent coefficients enter our abstract framework.

Example 1. Let $\Omega \in \mathbb{R}^d$ be a bounded domain with smooth boundary. We consider the linear parabolic initial-boundary value problem

$$\frac{\partial U}{\partial t}(x,t) = \mathscr{A}(x,t)U(x,t) + f(x,t), \quad x \in \Omega, \quad 0 < t \leqslant T \tag{11a}$$

with homogeneous Dirichlet boundary conditions and initial condition

$$U(x,0) = U_0(x), \quad x \in \Omega. \tag{11b}$$

Here, $\mathscr{A}(x,t)$ is a second-order strongly elliptic differential operator

$$\mathscr{A}(x,t) = \sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\left(\alpha_{ij}(x,t)\frac{\partial}{\partial x_j}\right) + \sum_{i=1}^{d} \beta_i(x,t)\frac{\partial}{\partial x_i} + \gamma(x,t). \tag{11c}$$

We require that the time-dependent coefficients α_{ij}, β_i, and γ are smooth functions of the variable $x \in \overline{\Omega}$ and Hölder-continuous with respect to t. For $1 < p < \infty$ and $\psi \in C_0^\infty(\Omega)$, we set $(A_p(t)\psi)(x) = \mathscr{A}(x,t)\psi(x)$ and consider $A_p(t)$ as an unbounded operator on $L^p(\Omega)$. It is well-known that this operator satisfies Hypotheses 1 and 2 with

$$X = L^p(\Omega) \quad \text{and} \quad D_p = W^{2,p}(\Omega) \cap W_0^{1,p}(\Omega), \tag{11d}$$

see [14, Section 7.6, 15, Section 5.2].

Our aim is to analyse the convergence behaviour of (8) for parabolic problems (1). Section 3 is concerned with the derivation of the needed stability results.

3. Stability

In order to study the stability properties of the Magnus integrator (8), it suffices to consider the homogeneous equation under discretisation. Resolving recursion (7) yields

$$u_{n+1} = \prod_{i=0}^{n} \mathrm{e}^{hA_i} u_0 \quad \text{for } n \geqslant 0.$$

Here, for noncommutative operators F_i on a Banach space the product is defined by

$$\prod_{i=m}^{n} F_i = \begin{cases} F_n F_{n-1} \cdots F_m & \text{if } n \geqslant m, \\ I & \text{if } n < m. \end{cases}$$

In the sequel, we derive bounds for the discrete evolution operator

$$\prod_{i=m}^{n} \mathrm{e}^{hA_i} \quad \text{for } n > m \geqslant 0 \tag{12}$$

in different norms. In Theorem 1, for notational simplicity, we do not distinguish the appearing constants.

Theorem 1 (*Stability*). *Under Hypotheses* 1–2 *the bounds*

$$\left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} \right\|_{X \leftarrow X} \leqslant M_5 \quad \text{and} \quad \left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} \right\|_{D \leftarrow X} \leqslant M_5 (t_{n+1} - t_m)^{-1} (1 + (1 + |\log h|)(t_{n+1} - t_m)^{\alpha})$$

are valid for $0 \leqslant t_m < t_n \leqslant T$ *with constant* $M_5 \geqslant 1$ *not depending on n and h.*

Proof. For proving the above stability bounds, our techniques are close to that used in [13]. The needed auxiliary estimates are given in Lemma 1 at the end of this section.

The main idea is to compare the discrete evolution operator (12) with the frozen operator

$$\prod_{i=m}^{n} \mathrm{e}^{hA_m} = \mathrm{e}^{(t_{n+1} - t_m)A_m},$$

where (5) applies directly. Therefore, it remains to estimate the difference

$$\Delta_m^n = \prod_{i=m}^{n} \mathrm{e}^{hA_i} - \prod_{i=m}^{n} \mathrm{e}^{hA_m}.$$

From a telescopic identity, it follows

$$\Delta_m^n = \sum_{j=m+1}^{n-1} \Delta_{j+1}^n (\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) \mathrm{e}^{(t_j - t_m)A_m} + \sum_{j=m+1}^{n} \mathrm{e}^{(t_{n+1} - t_{j+1})A_m} (\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) \mathrm{e}^{(t_j - t_m)A_m}. \tag{13}$$

(i) We first estimate Δ_m^n as operator from X to X. An application of Lemma 1 and relation (5) yields

$$\begin{aligned} \|\Delta_m^n\|_{X \leftarrow X} \leqslant & \sum_{j=m+1}^{n-1} \|\Delta_{j+1}^n\|_{X \leftarrow X} \|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) \mathrm{e}^{(t_j - t_m)A_m}\|_{X \leftarrow X} \\ & + \sum_{j=m+1}^{n} \|\mathrm{e}^{(t_{n+1} - t_{j+1})A_m}\|_{X \leftarrow X} \|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) \mathrm{e}^{(t_j - t_m)A_m}\|_{X \leftarrow X} \\ & \leqslant Ch \sum_{j=m+1}^{n-1} \|\Delta_{j+1}^n\|_{X \leftarrow X} (t_j - t_m)^{-1+\alpha} + Ch \sum_{j=m+1}^{n} (t_j - t_m)^{-1+\alpha} \end{aligned}$$

with some constant $C > 0$ depending on M_2 and M_6. Interpreting the second sum as a Riemann-sum and bounding it by the corresponding integral shows

$$\|\Delta_m^n\|_{X\leftarrow X} \leqslant Ch \sum_{j=m+1}^{n-1} \|\Delta_{j+1}^n\|_{X\leftarrow X}(t_j - t_m)^{-1+\alpha} + C,$$

where the constant additionally depends on T, see also [13]. A Gronwall-type inequality implies

$$\|\Delta_m^n\|_{X\leftarrow X} \leqslant C, \tag{14}$$

and, with the help of (5), the desired estimate for the discrete evolution operator follows:

$$\left\|\prod_{i=m}^{n} \mathrm{e}^{hA_i}\right\|_{X\leftarrow X} \leqslant \|\Delta_m^n\|_{X\leftarrow X} + \|\mathrm{e}^{(t_{n+1}-t_m)A_m}\|_{X\leftarrow X} \leqslant M_5.$$

(ii) For estimating $\|\Delta_m^n\|_{D\leftarrow X}$, we consider (13) and apply once more Lemma 1 and relation (5)

$$\begin{aligned}\|\Delta_m^n\|_{D\leftarrow X} \leqslant\ & \sum_{j=m+1}^{n-1} \|\Delta_{j+1}^n\|_{D\leftarrow X}\|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_j-t_m)A_m}\|_{X\leftarrow X} \\ & + \sum_{j=m+1}^{n-1} \|\mathrm{e}^{(t_{n+1}-t_{j+1})A_m}\|_{D\leftarrow X}\|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_j-t_m)A_m}\|_{X\leftarrow X} \\ & + \|(\mathrm{e}^{hA_n} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_n-t_m)A_m}\|_{D\leftarrow X} \\ \leqslant\ & Ch \sum_{j=m+1}^{n-1} \|\Delta_{j+1}^n\|_{D\leftarrow X}(t_j - t_m)^{-1+\alpha} + Ch \sum_{j=m+1}^{n-1} (t_{n+1} - t_{j+1})^{-1}(t_j - t_m)^{-1+\alpha} \\ & + C(t_n - t_m)^{-1+\alpha}.\end{aligned}$$

We estimate the Riemann-sum by the corresponding integral and apply a Gronwall inequality, see [12]. This yields

$$\|\Delta_m^n\|_{D\leftarrow X} \leqslant C(1 + |\log h|)(t_{n+1} - t_m)^{-1+\alpha}.$$

Together with (5) we finally obtain the desired result. □

The following auxiliary result is needed in the proof of Theorem 1.

Lemma 1. *In the situation of Theorem* 1, *the estimates*

$$\|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_j-t_m)A_m}\|_{X\leftarrow X} \leqslant M_6 h(t_j - t_m)^{-1+\alpha} \quad \textit{and}$$
$$\|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_j-t_m)A_m}\|_{D\leftarrow X} \leqslant M_6(t_j - t_m)^{-1+\alpha}$$

are valid for $0 \leqslant t_m < t_j \leqslant T$ *with some constant* $M_6 > 0$ *not depending on n and h.*

Proof. For proving Lemma 1, we employ standard techniques, see e.g., [10, Proof of Prop. 2.1.1].

Let Γ be a path surrounding the spectrum of the sectorial operators A_j and A_m. By means of the integral formula of Cauchy, the representation

$$
\begin{aligned}
(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m})\mathrm{e}^{(t_j-t_m)A_m} &= \frac{1}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^\lambda ((\lambda - hA_j)^{-1} - (\lambda - hA_m)^{-1})\, \mathrm{e}^{(t_j-t_m)A_m}\, \mathrm{d}\lambda \\
&= \frac{1}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^\lambda (\lambda - hA_j)^{-1} h(A_j - A_m)(\lambda - hA_m)^{-1} \mathrm{e}^{(t_j-t_m)A_m}\, \mathrm{d}\lambda \qquad (15)
\end{aligned}
$$

follows. The main tools for estimating this relation are the resolvent bound (2), estimate (5) and the Hölder property (6). We omit the details. □

4. Convergence

In the following, we analyse the convergence behaviour of the Magnus integrator (8) for (1). For that purpose, we next derive a representation of the global error.

We consider the initial value problem (1) on a subinterval $[t_n, t_{n+1}]$ and rewrite the right-hand side of the equation as follows:

$$u'(t) = A(t)u(t) + b(t) = A_n u(t) + b_n + g_n(t),$$

where the map g_n is defined by

$$g_n(t) = (A(t) - A_n)u(t) + b(t) - b_n \quad \text{for } t_n \leqslant t \leqslant t_{n+1}. \qquad (16)$$

Consequently, by the variation-of-constants formula, we obtain the following representation of the exact solution:

$$u(t_{n+1}) = \mathrm{e}^{hA_n} u(t_n) + \int_0^h \mathrm{e}^{(h-\tau)A_n} (b_n + g_n(t_n + \tau))\, \mathrm{d}\tau. \qquad (17)$$

On the other hand, the numerical solution is given by relation (8), see also (9). Let $e_{n+1} = u_{n+1} - u(t_{n+1})$ denote the error at time t_{n+1} and δ_{n+1} the corresponding defect

$$\delta_{n+1} = \int_0^h \mathrm{e}^{(h-\tau)A_n} g_n(t_n + \tau)\, \mathrm{d}\tau. \qquad (18)$$

By taking the difference of (8) and (17), we thus obtain

$$e_{n+1} = \mathrm{e}^{hA_n} e_n - \delta_{n+1}, \quad n \geqslant 0, \quad e_0 = 0.$$

Resolving this error recursion finally yields

$$e_n = -\sum_{j=0}^{n-1} \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \delta_{j+1}, \quad n \geqslant 1, \quad e_0 = 0.$$

For the subsequent convergence analysis, it is useful to employ an expansion of the defects which we derive in the following.

Provided that the map g_n is twice differentiable on (t_n, t_{n+1}), we obtain from a Taylor series expansion

$$g_n(t_n+\tau) = \left(\tau - \frac{h}{2}\right) g_n'\left(t_n + \frac{h}{2}\right) + \left(\tau - \frac{h}{2}\right)^2 \int_0^1 (1-\sigma) g_n''\left(t_n + \frac{h}{2} + \sigma\left(\tau - \frac{h}{2}\right)\right) \mathrm{d}\sigma,$$

where $0 < \tau < h$. We insert this expansion into (18) and express the terms involving g_n' with the help of the bounded linear operators

$$\varphi(hA_n) = \frac{1}{h}\int_0^h \mathrm{e}^{(h-\tau)A_n}\,\mathrm{d}\tau \quad \text{and} \quad \psi(hA_n) = \frac{1}{h^2}\int_0^h \mathrm{e}^{(h-\tau)A_n}\,\tau\,\mathrm{d}\tau. \tag{19}$$

Thus, we obtain the following representation of the defects

$$\begin{aligned}\delta_{n+1} = {} & h^2\left(\psi(hA_n) - \frac{1}{2}\varphi(hA_n)\right) g_n'\left(t_n + \frac{h}{2}\right) \\ & + \int_0^h \mathrm{e}^{(h-\tau)A_n}\left(\tau - \frac{h}{2}\right)^2 \int_0^1 (1-\sigma)\, g_n''\left(t_n + \frac{h}{2} + \sigma\left(\tau - \frac{h}{2}\right)\right) \mathrm{d}\sigma\,\mathrm{d}\tau.\end{aligned}$$

For later it is also substantial that the equality

$$\psi(hA_n) - \tfrac{1}{2}\varphi(hA_n) = hA_n\chi(hA_n)$$

holds with some bounded linear operator $\chi(hA_n)$. Precisely, after possibly enlarging the constant $M_4 \geqslant 1$ in (10), we receive

$$\begin{aligned}&\|\varphi(hA_n)\|_{X\leftarrow X} + \|\varphi(hA_n)\|_{D\leftarrow D} + \|\psi(hA_n)\|_{X\leftarrow X} \\ &\quad + \|\psi(hA_n)\|_{D\leftarrow D} + \|\chi(hA_n)\|_{X\leftarrow X} + \|\chi(hA_n)\|_{D\leftarrow D} \leqslant M_4.\end{aligned} \tag{20}$$

The bounds for $\varphi(hA_n)$ and $\psi(hA_n)$ are a direct consequence of the defining relations (19) and (5), see also (10), whereas the boundedness of $\chi(hA_n)$ follows by means of the integral formula of Cauchy.

We first specify a convergence estimate under the assumption that the true solution of (1) possesses favourable regularity properties. Our main tool for the derivation of this error bound is the stability result stated in Section 3. In view of the proof of our convergence result, it is convenient to introduce several abbreviations. Accordingly to the above considerations, we split the defects $\delta_{j+1} = \delta_{j+1}^{(1)} + \delta_{j+1}^{(2)}$ where

$$\begin{aligned}\delta_{j+1}^{(1)} &= h^2\left(\psi(hA_j) - \frac{1}{2}\varphi(hA_j)\right) g_j'\left(t_j + \frac{h}{2}\right) = h^3 A_j\chi(hA_j) g_j'\left(t_j + \frac{h}{2}\right), \\ \delta_{j+1}^{(2)} &= \int_0^h \mathrm{e}^{(h-\tau)A_j}\left(\tau - \frac{h}{2}\right)^2 \int_0^1 (1-\sigma)\, g_j''\left(t_j + \frac{h}{2} + \sigma\left(\tau - \frac{h}{2}\right)\right) \mathrm{d}\sigma\,\mathrm{d}\tau.\end{aligned} \tag{21a}$$

Analogously, the error is decomposed into $e_n = -e_n^{(1)} - e_n^{(2)}$ with

$$e_n^{(k)} = \sum_{j=0}^{n-1} \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i}\,\delta_{j+1}^{(k)}, \quad k = 1, 2. \tag{21b}$$

Henceforth, we denote by $\|g_n\|_{X,\infty} = \max\{\|g_n(t)\|_X \,:\, t_n \leqslant t \leqslant t_{n+1}\}$ the maximum value of the map $g_n = (A - A_n)u + b - b_n$ on the interval $[t_n, t_{n+1}]$. Recall the abbreviations $A_n = A(t_n + h/2)$ and $b_n = b(t_n + (h/2))$ introduced in (7) and (8). Further, we set

$$\|g\|_{X,\infty} = \max\{\|g_n\|_{X,\infty} : n \geqslant 0,\ t_{n+1} \leqslant T\}.$$

Theorem 2 (*Convergence*). *Under Hypotheses* 1–2 *with* $\alpha = 1$, *apply the Magnus integrator* (8) *to the initial value problem* (1). *Then, the convergence estimate*

$$\|u_n - u(t_n)\|_X \leqslant Ch^2(\|g'\|_{D,\infty} + \|g''\|_{X,\infty}),$$

is valid for $0 \leqslant t_n \leqslant T$, *provided that the quantities on the right-hand side are well-defined. The constant* $C > 0$ *does not depend on n and h.*

Proof. We successively consider the error terms $e_n^{(1)}$ and $e_n^{(2)}$ specified above. An application of Theorem 1 yields

$$\begin{aligned}
\|e_n^{(1)}\|_X &\leqslant \left\| \sum_{j=0}^{n-2} \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \delta_{j+1}^{(1)} \right\|_X + \|\delta_n^{(1)}\|_X \\
&\leqslant h^2 \cdot h \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \right\|_{X \leftarrow X} \|A_j\|_{X \leftarrow D} \|\chi(hA_j)\|_{D \leftarrow D} \left\| g_j'\left(t_j + \frac{h}{2}\right) \right\|_D \\
&\quad + h^2(\|\varphi(hA_{n-1})\|_{X \leftarrow X} + \|\psi(hA_{n-1})\|_{X \leftarrow X}) \left\| g_{n-1}'\left(t_{n-1} + \frac{h}{2}\right) \right\|_X \\
&\leqslant C\|g'\|_{D,\infty} h^2
\end{aligned}$$

with $C > 0$ depending on the constants M_5 and M_4 appearing in Theorem 1 and (20), on $\|A(t)\|_{X \leftarrow D}$, and on T. A direct estimation of $\delta_{j+1}^{(2)}$ with the help of (5) shows

$$\begin{aligned}
\|\delta_{j+1}^{(2)}\|_X &\leqslant \int_0^h \|\mathrm{e}^{(h-\tau)A_j}\|_{X \leftarrow X} \left(\tau - \frac{h}{2}\right)^2 \int_0^1 (1-\sigma) \left\| g_j''\left(t_j + \frac{h}{2} + \sigma\left(\tau - \frac{h}{2}\right)\right) \right\|_X \mathrm{d}\sigma\, \mathrm{d}\tau \\
&\leqslant M_2 \|g''\|_{X,\infty} h^3.
\end{aligned}$$

Consequently, for the remaining term, we obtain by Theorem 1

$$\|e_n^{(2)}\|_X \leqslant \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \right\|_{X \leftarrow X} \|\delta_{j+1}^{(2)}\|_X + \|\delta_n^{(2)}\|_X \leqslant C\|g''\|_{X,\infty} h^2$$

with a constant $C > 0$ depending on M_2, M_5, and T. Altogether, the desired estimate follows. □

We remark that, in the situation of the theorem, Hypothesis 2 is always fulfilled with $\alpha = 1$. However, in view of applications, the condition on the derivative of g_n is often too restrictive. We next prove a convergence result under weaker assumptions on g_n'. For the proof of Theorem 3 an extension of our stability result is needed which we give at the end of this section.

Theorem 3 (*Convergence*). *Under Hypotheses* 1–2 *with* $\alpha = 1$, *the Magnus integrator* (8) *applied to* (1) *satisfies the bound*

$$\|u_n - u(t_n)\|_X \leqslant Ch^2((1 + |\log h|)\|g'\|_{X,\infty} + \|g''\|_{X,\infty})$$

for $0 \leqslant t_n \leqslant T$ *with some constant* $C > 0$ *not depending on n and h.*

Proof. Following the proof of Theorem 2, we show a refined error estimate for $e_n^{(1)}$. Due to Lemma 2 which is given at the end of this section, we have

$$\begin{aligned}\|e_n^{(1)}\|_X \leqslant{}& h^2 \cdot h \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} A_j \chi(hA_j) \right\|_{X \leftarrow X} \left\| g_j'\left(t_j + \frac{h}{2}\right)\right\|_X \\ &+ h^2(\|\varphi(hA_{n-1})\|_{X\leftarrow X} + \|\psi(hA_{n-1})\|_{X\leftarrow X}) \left\| g_{n-1}'\left(t_{n-1} + \frac{h}{2}\right)\right\|_X \\ \leqslant{}& C\|g'\|_{X,\infty} h^2(1 + |\log h|)\end{aligned}$$

which yields the result of the theorem. □

In the sequel, we analyse the convergence behaviour of (8) with respect to the norm in D. For that purpose, we introduce the notion of intermediate spaces, see also [10].

For some $0 < \vartheta < 1$ let $X_\vartheta = (X, D)_{\vartheta,p}$ denote the real interpolation space between X and D. Consequently, the norm in X_ϑ fulfills the relation

$$\|x\|_{X_\vartheta} \leqslant C_v \|x\|_D^\vartheta \|x\|_X^{1-\vartheta} \quad \text{for all } x \in D$$

with some constant $C_v > 0$. In particular, it follows

$$\|\mathrm{e}^{tA(s)}\|_{X_\vartheta \leftarrow X_\vartheta} + \|t^{1-\vartheta}\mathrm{e}^{tA(s)}\|_{D\leftarrow X_\vartheta} \leqslant M_2 \quad \text{for } 0 \leqslant t \leqslant T. \tag{22}$$

For the subsequent derivations, we choose ϑ in such a way that the interpolation space $X_{1+\vartheta} = (D, D(A(t)^2))_{\vartheta,p}$ between D and the domain of $A(t)^2$ is independent of t, and that the map A satisfies a Lipschitz-condition from $X_{1+\vartheta}$ to X_ϑ. In applications, this assumption is fulfilled for ϑ sufficiently small, see also Example 2.

Hypothesis 3. For some $0 < \vartheta < 1$, the interpolation space $X_{1+\vartheta}$ does not depend on t. Further, we suppose that the estimate

$$\|A(t) - A(s)\|_{X_\vartheta \leftarrow X_{1+\vartheta}} \leqslant M_3(t - s)$$

holds with some constant $M_3 > 0$ for all $0 \leqslant s \leqslant t \leqslant T$.

In this situation, following the proof of Theorem 1, we obtain

$$\left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} \right\|_{X_\vartheta \leftarrow X_\vartheta} \leqslant M_5 \quad \text{and} \quad \left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} \right\|_{D \leftarrow X_\vartheta} \leqslant M_5 (t_{n+1} - t_m)^{-1+\vartheta}, \tag{23}$$

after a possible enlargement of $M_5 \geqslant 1$.

Example 2. In continuation of Example 1, we consider the second-order parabolic partial differential equation (11) subject to homogeneous Dirichlet boundary conditions and a certain initial condition. For this initial-boundary value problem, the admissible value of ϑ in Hypothesis 3 relies on the characterisation of the interpolation spaces between $D = W^{2,p}(\Omega) \cap W_0^{1,p}(\Omega)$ and $D(A(t)^2)$. It follows from [4, Théorème 8.1′] that for $0 \leqslant \vartheta < 1/(2p)$ the interpolation space $X_{1+\vartheta}$ is isomorphic to $W^{2+2\vartheta,p}(\Omega) \cap W_0^{1,p}(\Omega)$ and thus independent of t. This is no longer true for $\vartheta > 1/(2p)$, since $X_{1+\vartheta}$, in general, depends on t through the boundary conditions $A(t)u = 0$ on $\partial\Omega$. Therefore, we may choose $0 \leqslant \vartheta < 1/(2p)$ in Hypothesis 3. Assuming that the spatial derivatives of the coefficients α_{ij}, β_i, and γ are Hölder continuous with respect to t, the required Hölder continuity of $A(t)$ on $X_{1+\vartheta}$ follows.

Under the requirement that the first derivative of g_n is bounded in D and that g_n'' belongs to the interpolation space X_γ for some $\gamma > 0$ arbitrarily small, the following result is valid. Note that for stepsizes $h > 0$ sufficiently small it follows $\gamma^{-1} h^\gamma \leqslant C|\log h|$.

Theorem 4. *Suppose that Hypotheses* 1–2 *with* $\alpha = 1$ *and Hypothesis* 3 *with* $\vartheta = \gamma$ *are fulfilled and apply the Magnus integrator* (8) *to the initial value problem* (1). *Then, the convergence estimate*

$$\|u_n - u(t_n)\|_D \leqslant Ch^2((1 + |\log h|)\|g'\|_{D,\infty} + (1 + \gamma^{-1}h^\gamma)\|g''\|_{X_\gamma,\infty})$$

holds true for $0 \leqslant t_n \leqslant T$. *The constant* $C > 0$ *is independent of n and h.*

Proof. Similarly as in the proof of Theorem 2, we successively analyse the error terms $e_n^{(1)}$ and $e_n^{(2)}$ defined in (21) by applying Theorem 1 and (20). On the one hand, we receive

$$\begin{aligned}
\|e_n^{(1)}\|_D &\leqslant \left\| \sum_{j=0}^{n-2} \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \delta_{j+1}^{(1)} \right\|_D + \|\delta_n^{(1)}\|_D \\
&\leqslant h^2 \cdot h \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \right\|_{D \leftarrow X} \|A_j\|_{X \leftarrow D} \|\chi(hA_j)\|_{D \leftarrow D} \left\| g_j' \left(t_j + \frac{h}{2} \right) \right\|_D \\
&\quad + h^2 (\|\varphi(hA_{n-1})\|_{D \leftarrow D} + \|\psi(hA_{n-1})\|_{D \leftarrow D}) \left\| g_{n-1}' \left(t_{n-1} + \frac{h}{2} \right) \right\|_D \\
&\leqslant C\|g'\|_{D,\infty} h^2 (1 + |\log h|).
\end{aligned}$$

A direct estimation of $\delta_{j+1}^{(2)}$ with the help of the relation (22) shows

$$\begin{aligned}
\|\delta_{n+1}^{(2)}\|_{X_\gamma} &\leqslant \int_0^h \|\mathrm{e}^{(h-\tau)A_n}\|_{X_\gamma \leftarrow X_\gamma} \left(\tau - \frac{h}{2} \right)^2 \int_0^1 (1 - \sigma) \left\| g_n'' \left(t_n + \frac{h}{2} + \sigma \left(\tau - \frac{h}{2} \right) \right) \right\|_{X_\gamma} \mathrm{d}\sigma \, \mathrm{d}\tau \\
&\leqslant M_2 \|g''\|_{X_\gamma,\infty} h^3.
\end{aligned}$$

Besides, we receive

$$\begin{aligned}
\|\delta_{j+1}^{(2)}\|_D &\leqslant \int_0^h \|\mathrm{e}^{(h-\tau)A_j}\|_{D \leftarrow X_\gamma} \left(\tau - \frac{h}{2} \right)^2 \int_0^1 (1 - \sigma) \left\| g_j'' \left(t_j + \frac{h}{2} + \sigma \left(\tau - \frac{h}{2} \right) \right) \right\|_{X_\gamma} \mathrm{d}\sigma \, \mathrm{d}\tau \\
&\leqslant M_2 \|g''\|_{X_\gamma,\infty} \gamma^{-1} h^{2+\gamma}.
\end{aligned}$$

Consequently, together with (23) it follows

$$
\begin{aligned}
\|e_n^{(2)}\|_D &\leqslant \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} \right\|_{D\leftarrow X_\gamma} \|\delta_{j+1}^{(2)}\|_{X_\gamma} + \|\delta_n^{(2)}\|_D \\
&\leqslant C\|g''\|_{X_\gamma,\infty}\, h^2(1+\gamma^{-1}h^\gamma).
\end{aligned}
$$

This yields the given result. □

We next extend the above result to the situation where the first derivative of g belongs to the interpolation space $X_\beta = (X, D)_{\beta,p}$ for some $0 < \beta < 1$. If Hypothesis 3 holds with $\vartheta = \beta$, a proof similar to that of Lemma 2 below yields the auxiliary estimate

$$
\left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} A_{m-1}\chi(hA_{m-1}) \right\|_{D\leftarrow X_\beta} \leqslant M_5 h^{-1+\beta}(t_{n+1}-t_m)^{-1}. \tag{24}
$$

As before, we further suppose $g_n'' \in X_\gamma$ for some $\gamma > 0$ arbitrarily small. Maximising the term $\gamma^{-1}h^\gamma$ with respect to γ yields $\gamma^{-1}h^\gamma \leqslant C|\log h|$ for $h > 0$ sufficiently small.

Theorem 5. *Under Hypotheses* 1–2 *with* $\alpha = 1$ *and Hypothesis* 3 *with* $\vartheta = \beta$, *the Magnus integrator* (8) *for* (1) *satisfies the estimate*

$$
\|u_n - u(t_n)\|_D \leqslant C(h^{1+\beta}(1+|\log h|)\|g'\|_{X_\beta,\infty} + h^2(1+\gamma^{-1}h^\gamma)\|g''\|_{X_\gamma,\infty})
$$

for $0 \leqslant t_n \leqslant T$ *with some constant* $C > 0$ *independent of* n *and* h.

Proof. We follow the proof of Theorem 4 and modify the estimation of $e_n^{(1)}$. If $g' \in X_\beta$ the integral formula of Cauchy implies

$$
\begin{aligned}
\|\delta_n^{(1)}\|_D &\leqslant h^2 \left\| \psi(hA_{n-1}) - \frac{1}{2}\,\varphi(hA_{n-1}) \right\|_{D\leftarrow X_\beta} \left\| g_{n-1}'\left(t_{n-1}+\frac{h}{2}\right)\right\|_{X_\beta} \\
&\leqslant Ch^{1+\beta}\|g'\|_{X_\beta}.
\end{aligned}
$$

Together with (24) we thus receive

$$
\begin{aligned}
\|e_n^{(1)}\|_D &\leqslant \left\| \sum_{j=0}^{n-2} \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i}\delta_{j+1}^{(1)} \right\|_D + \|\delta_n^{(1)}\|_D \\
&\leqslant h^2 \cdot h \sum_{j=0}^{n-2} \left\| \prod_{i=j+1}^{n-1} \mathrm{e}^{hA_i} A_j\chi(hA_j) \right\|_{D\leftarrow X_\beta} \left\| g_j'\left(t_j+\frac{h}{2}\right)\right\|_{X_\beta} \\
&\quad + h^2 \left\| \psi(hA_{n-1}) - \frac{1}{2}\,\varphi(hA_{n-1}) \right\|_{D\leftarrow X_\beta} \left\| g_{n-1}'\left(t_{n-1}+\frac{h}{2}\right)\right\|_{X_\beta} \\
&\leqslant C\|g'\|_{X_\beta,\infty}\, h^{1+\beta}(1+|\log h|)
\end{aligned}
$$

which yields the given result. □

The following extension of Theorem 1 is needed in the proof of Theorem 3.

Lemma 2. *Assume that Hypotheses* 1–2 *with* $\alpha = 1$ *hold. Then, the bound*

$$\left\| \prod_{i=m}^{n} \mathrm{e}^{hA_i} A_{m-1}\chi(hA_{m-1}) \right\|_{X\leftarrow X} \leqslant M_5(1 + |\log h| + (t_{n+1} - t_m)^{-1}) \tag{25}$$

is valid for $0 \leqslant t_m < t_n \leqslant T$ *with some constant* $M_5 > 0$ *not depending on n and h.*

Proof. We note that by the integral formula of Cauchy, Theorem 1 and Hypotheses 1–2 it suffices to prove the desired bound (25) with A_{m-1} replaced by A_m. Thus, as in the proof of Theorem 1, we compare the discrete evolution operator with a frozen operator

$$\prod_{i=m}^{n} \mathrm{e}^{hA_i} A_m\chi(hA_m) = \Delta_m^n A_m\chi(hA_m) + A_m \mathrm{e}^{(t_{n+1}-t_m)A_m}\chi(hA_m).$$

Clearly, the second term is bounded by

$$\|A_m \mathrm{e}^{(t_{n+1}-t_m)A_m}\|_{X\leftarrow X}\|\chi(hA_m)\|_{X\leftarrow X} \leqslant C(t_{n+1} - t_m)^{-1},$$

see (5) and remark above as well as (20). For estimating the first term, we employ relation (13) for Δ_m^n given in the proof of Theorem 1 and receive

$$\begin{aligned}\Delta_m^n A_m\chi(hA_m) = &\sum_{j=m+1}^{n-1} \Delta_{j+1}^n (\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) A_m \mathrm{e}^{(t_j-t_m)A_m}\chi(hA_m)\\ &+ \sum_{j=m+1}^{n} \mathrm{e}^{(t_{n+1}-t_{j+1})A_m}(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) A_m \mathrm{e}^{(t_j-t_m)A_m}\chi(hA_m).\end{aligned}$$

As a consequence of the integral formula of Cauchy, see also (15), we obtain

$$\|(\mathrm{e}^{hA_j} - \mathrm{e}^{hA_m}) A_m \mathrm{e}^{(t_j-t_m)A_m}\|_{X\leftarrow X} \leqslant Ch(t_j - t_m)^{-1}.$$

Together with (5), (14) and (20), it thus follows

$$\|\Delta_m^n A_m\chi(hA_m)\|_{X\leftarrow X} \leqslant Ch \sum_{j=m+1}^{n} (t_j - t_m)^{-1} \leqslant C(1 + |\log h|).$$

Altogether, this proves the desired result. □

5. Numerical examples

In order to illustrate the sharpness of the proven orders in our convergence bounds, we consider problem (11) in one space dimension for $x \in [0, 1]$ and $t \in [0, 1]$. We choose $\alpha(x, t) = 1 + \mathrm{e}^{-t}$ and $\beta(x, t) = \gamma(x, t) = 0$, and we determine $f(x, t)$ in such a way that the exact solution is given by $U(x, t) = x(1 - x)\mathrm{e}^{-t}$.

Table 1
Numerically observed temporal orders of convergence in different norms for discretisations with N spatial degrees of freedom and time stepsize $h = 1/128$

N	D_1	D_2	D_∞	L^1	L^2	L^∞
50	1.624	1.375	1.217	1.981	1.986	2.000
100	1.562	1.310	1.101	1.979	1.986	1.998
200	1.531	1.280	1.051	1.979	1.986	1.998
300	1.521	1.270	1.034	1.979	1.986	1.998
400	1.516	1.266	1.026	1.979	1.986	1.998

We discretise the partial differential equation in space by standard finite differences and in time by the Magnus integrator (8), respectively. Due to the particular form of the exact solution, the spatial discretisation error of our method is zero. The numerically observed temporal orders of convergence in various discrete norms are shown in Table 1. Recall that $X = L^p(\Omega)$ and $D_p = W^{2,p}(\Omega) \cap W_0^{1,p}(\Omega)$.

The numerically observed order in the discrete L^2-norm is approximately 2, which is in accordance with Theorem 3. There is further a pronounced order reduction to approximately 1.25 in the discrete D_2-norm for sufficiently large N. This is explained as follows. The attainable value of β in Theorem 5 is restricted on the one hand by Hypothesis 3 and on the other hand by the domain of the function

$$g_n'(t) = A'(t)u(t) + (A(t) - A_n)u'(t) + b'(t), \quad t_n \leqslant t \leqslant t_{n+1},$$

see (16). In our example, g_n' is spatially smooth but does not satisfy the boundary conditions. For $X = L^2(\Omega)$ the optimal value is therefore $\beta = 1/4 - \varepsilon$ for arbitrarily small $\varepsilon > 0$, see [3,4] and the discussion in Example 2.

Similarly, for arbitrary $1 < p < \infty$, Theorem 3 predicts order 2 for the L^p-error, whereas an order reduction to approximately $1 + 1/(2p)$ in the discrete D_p-norm for large N is explained by Theorem 5. These numbers are in perfect agreement with Table 1, where we illustrated the limit cases $p = 1$ and $p = \infty$.

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