A second-order Magnus type integrator for non-autonomous semilinear parabolic problems

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Keywords

Semilinear parabolic problems; Time-dependent coefficients; Magnus integrators; Exponential integrators; Stability; Convergence

Abstract

In this note, we proceed the stability and convergence analysis of Magnus type integrators for the time discretisation of parabolic partial differential equations with time-dependent coefficients and consider a second-order method for semilinear problems. The error analysis given is a step towards the construction and study of an explicit exponential integration scheme for quasilinear parabolic problems.

Employing an abstract formulation of a parabolic initial-boundary value problem as an initial value problem on a function space, we work within the framework of sectorial operators and analytic semigroups on Banach spaces. Under reasonable requirements on the smoothness of the data and the exact solution, we derive an error estimate in the domain of the nonlinearity. The theoretical result is illustrated by a numerical example.

1 Introduction

In this paper, we analyse the error behaviour of a Magnus type integrator for non-autonomous differential equations of the form

$$u'(t) = A(t)u(t) + b\big(t, u(t)\big), \quad 0 < t \le T, \qquad u(0) = u_0. \tag{1.1}$$

The abstract framework is based on the theory of sectorial operators and analytic semigroups on Banach spaces and includes semilinear parabolic initial-boundary value problems with time-dependent coefficients.

The present work proceeds González et al. [5], where we considered linear non-autonomous problems

$$u'(t) = A(t)u(t) + b(t), \quad 0 < t \le T, \qquad u(0) = u_0, \tag{1.2}$$

and studied a mixed method that integrates the homogeneous part by a second-order Magnus integrator and the inhomogeneous part by the exponential midpoint

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rule. Under reasonable requirements on the smoothness of the data and the exact solution, we proved a second-order convergence estimate with respect to the norm of the underlying function space, avoiding unnatural restrictions on the time stepsize.

The mixed method for (1.2) is now extended to semilinear equations (1.1) in such a way that the resulting scheme is of classical order 2. Thereby, similarly as for explicit exponential Runge–Kutta methods, the numerical approximation is determined by means of an additional internal stage. The main benefit of the numerical scheme is that the nonlinearity is integrated explicitely.

The contents of the paper are as follows. In Section 2, we state the basic assumptions on the problem class and collect several auxiliary definitions and results. As an illustration, we specify a parabolic initial-boundary value problem under a boundary condition of Dirichlet type. The partial differential equation involves a second-order differential operator with regular space and time-dependent coefficients and a nonlinear function, which smoothly depends on the solution and its first-order space derivatives. We show that such problems, when considered as differential equations on L^p-spaces, are included in the abstract setting. In Section 3, we briefly introduce the concept of Magnus integrators and exponential Runge–Kutta methods and review some of the relevant literature in connection with stiff problems. This discussion also explains the definition of the numerical scheme for semilinear problems. The subsequent Section 4 contains stability bounds for the associated linear problem which are essential tools for the proof of the convergence result. Section 5 is devoted to the derivation of an error estimate with respect to the norm of the domain of the nonlinearity. This theoretical result implies that the order of convergence depends on the regularity properties of the data and the exact solution. Further, the order of convergence is effected by the function space in which the error is measured. If the domain of the nonlinear part involves additional boundary conditions, an order reduction is encountered, in general. The numerical example given in Section 6 confirms the predicted fractional convergence order in a discrete Sobolev-norm.

2 Problem class

In this section, we introduce the fundamental hypotheses on the abstract inital value problem (1.1), see also [5]. Besides, we collect several basic definitions and facts that are needed later for the statement of the numerical method and the proof of the main result. In our notation, we primarily follow the book of Lunardi [18]. For a detailed treatise of evolution equations and the theory of sectorial operators and analytic semigroups, we further refer to the monographs [9, 24, 26]. In order to simplify the notation, we do not distinguish the arising constants, i.e., the quantities $K > 0$ and $M > 0$ possibly take different values at different occurrences.

Henceforth, let $(X, \|\cdot\|_X)$ and $(D, \|\cdot\|_D)$ be Banach spaces with D densely embedded in X. The basic assumption on the map $A : [0, T] \to L(D, X)$ defining the right-hand side of (1.1) is the following.

Hypothesis 1 *The closed linear operator $A(t) : D \to X$ is uniformly sectorial for $t \in [0, T]$. That is, there exist constants $a \in \mathbb{R}$, $\phi \in (0, \pi/2)$, and $M > 0$ such that $A(t)$ satisfies the resolvent condition*

$$\left\| \big(\lambda I - A(t)\big)^{-1} \right\|_{X \leftarrow X} \leq \frac{M}{|\lambda - a|}, \qquad \lambda \in \mathbb{C} \setminus S_\phi(a), \tag{2.3}$$

where $S_\phi(a) = \big\{\lambda \in \mathbb{C} : \big|\arg(a-\lambda)\big| \le \phi\big\} \cup \{a\}$. *Furthermore, the graph norm of* $A(t)$ *and the norm in* D *are supposed to be equivalent. Thus, the relation*

$$K^{-1}\|x\|_D \le \|x\|_X + \big\|A(t)x\big\|_X \le K\|x\|_D, \qquad x \in D, \tag{2.4}$$

is valid for every $t \in [0,T]$ *with a constant* $K > 0$.

For any linear operator $F : X \to D$ estimate (2.4) implies

$$\big\|A(t)F\big\|_{X\leftarrow X} \le K\|F\|_{D\leftarrow X}, \qquad \|F\|_{D\leftarrow X} \le K\big(1 + \big\|A(t)F\big\|_{X\leftarrow X}\big). \tag{2.5}$$

Moreover, for fixed $s \in [0,T]$ the sectorial operator $S = A(s)$ generates an analytic semigroup $\big(\mathrm{e}^{tS}\big)_{t\ge 0}$ on X. The linear operator $\mathrm{e}^{tS} : X \to X$ is defined through the integral formula of Cauchy

$$\mathrm{e}^{tS} = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \mathrm{e}^{\lambda}\big(\lambda I - tS\big)^{-1}\,\mathrm{d}\lambda, \quad t > 0, \qquad \mathrm{e}^{tS} = I, \quad t = 0. \tag{2.6}$$

Here, Γ denotes a path that surrounds the spectrum of S. Consequently, with the help of (2.3) and (2.5), after possibly enlarging the constant $M > 0$, the bound

$$\big\|\mathrm{e}^{tS}\big\|_{X\leftarrow X} + \big\|\mathrm{e}^{tS}\big\|_{D\leftarrow D} + \big\|t\mathrm{e}^{tS}\big\|_{D\leftarrow X} \le M, \qquad 0 \le t \le T, \tag{2.7a}$$

follows, see also [18, Ch. 2].

The concept of intermediate spaces is essential in connection with semilinear parabolic problems. For $\vartheta \in (0,1)$ we denote by X_ϑ some intermediate space between $D = X_1$ and $X = X_0$ such that the norm in X_ϑ fulfills the relation

$$\|x\|_{X_\vartheta} \le K\|x\|_D^\vartheta \|x\|_X^{1-\vartheta}, \qquad x \in D,$$

with a constant $K > 0$. Examples are real interpolation spaces, see Lunardi [18], or fractional power spaces, see Henry [9]. As a consequence, the analytic semigroup satisfies the bound

$$\big\|\mathrm{e}^{tS}\big\|_{X_\vartheta\leftarrow X_\vartheta} + \big\|t^\vartheta \mathrm{e}^{tS}\big\|_{X_\vartheta\leftarrow X} \le M, \qquad 0 \le t \le T, \tag{2.7b}$$

with a constant $M > 0$. Furthermore, for $0 \le \mu \le \nu < 1$ it holds

$$\big\|t^{\nu-\mu}\mathrm{e}^{tS}\big\|_{X_\nu\leftarrow X_\mu} + \big\|t^{1+\nu-\mu} S\mathrm{e}^{tS}\big\|_{X_\nu\leftarrow X_\mu} \le M, \qquad 0 \le t \le T, \tag{2.7c}$$

see [18, Prop. 2.3.1].

In view of the proof of the stability result, we assume that $\vartheta \in [0,1)$ is chosen in such a way that the intermediate space $X_{1+\vartheta}$ between D and the domain of $A(t)^2$ is independent of the variable $t \in [0,T]$. Further, we need $A(t)$ to be Hölder-continuous with respect to t.

Hypothesis 2 *For some* $\vartheta \in [0,1)$ *the intermediate space* $X_{1+\vartheta}$ *does not depend on* $t \in [0,T]$. *Moreover, it holds* $A \in C^\alpha\big([0,T], L(X_{1+\vartheta}, X_\vartheta)\big)$ *with* $0 < \alpha \le 1$. *Thus, the estimate*

$$\big\|A(t) - A(s)\big\|_{X_\vartheta\leftarrow X_{1+\vartheta}} \le M(t-s)^\alpha, \qquad 0 \le s \le t \le T,$$

is valid with a constant $M > 0$.

The nonlinear map b on the right-hand side of (1.1) is defined on an intermediate space between X and D. Precisely, we suppose that for some $0 \leq \beta < 1$ it holds $b : [0,T] \times X_\beta \to X : (t,v) \mapsto b(t,v)$. This assumption together with Hypothesis 1 renders (1.1) a semilinear parabolic problem.

In view of Theorem 2, we need the map b to be differentiable with respect to the second variable v and its derivative $D_v b(t,v) : X_\beta \to X : w \mapsto D_v b(t,v)w$ to be bounded, uniformly for $0 \leq t \leq T$ and $v \in X_\beta$.

Hypothesis 3 *The derivative of the map $b : [0,T] \times X_\beta \to X$ with respect to v satisfies the bound*

$$\big\| D_v b(t,v) \big\|_{X \leftarrow X_\beta} \leq C, \qquad 0 \leq t \leq T, \qquad v \in X_\beta,$$

with some constant $C > 0$.

The following initial-boundary value problem can be cast into the abstract framework. Accordingly to Henry [9], X_ϑ denotes a fractional power space.

Example 1 Let Ω be a bounded domain in $\mathbb{R}^d$ with smooth boundary $\partial\Omega$. We consider the partial differential equation

$$\partial_t U(x,t) = \mathcal{A}(x,t)U(x,t) + f\big(x,t,U(x,t),\nabla U(x,t)\big), \quad x \in \Omega, \quad 0 < t \leq T,$$

subject to a homogeneous Dirichlet boundary condition and the initial condition $U(x,0) = U_0(x)$ for $x \in \Omega$. The second-order strongly elliptic differential operator

$$\mathcal{A}(x,t) = \sum_{i,j=1}^{d} \partial_{x_i}\big(\alpha_{ij}(x,t)\,\partial_{x_j}\big) + \sum_{i=1}^{d} \beta_i(x,t)\,\partial_{x_i} + \gamma(x,t)$$

involves the real-valued space and time-dependent coefficients α_{ij}, β_i, and γ which we assume to be sufficiently smooth on $\overline{\Omega} \times [0,T]$. In particular, we require that the spatial derivatives of the coefficients are Hölder-continuous with respect to t. The function f is supposed to be regular in all variables and to satisfy certain growth conditions, see Henry [9, Ex. 3.6] for the case $d = 1$ or Pazy [24, Th. 4.4] for $d = 3$.

In order to write this initial-boundary value problem as an initial value problem of the form (1.1) for $\big(u(t)\big)(x) = U(x,t)$, we define $A(t)v$ and $b(t,v)$ through

$$\big(A(t)v\big)(x) = \mathcal{A}(x,t)v(x), \qquad b(t,v)(x) = f\big(x,t,v(x),\nabla v(x)\big), \qquad v \in C_0^\infty(\Omega).$$

Then, $A(t)$ considered as an unbounded operator on the Hilbert space $X = L^2(\Omega)$ satisfies Hypothesis 1 with $D = H^2(\Omega) \cap H_0^1(\Omega)$. Moreover, for $d = 1$ we choose $X_\beta = X_{1/2}$ as the domain of the nonlinearity, whereas for $d = 3$ we require $\beta > 3/4$, see [9, 24].

A characterisation of the real interpolation spaces in Grisvard [7] implies that for $0 \leq \vartheta < 1/4$ no additional boundary condition will affect the intermediate space X_ϑ and that the interpolation spaces between D and $D\big(A(t)^2\big)$ are independent of the variable t. Contrary, for larger values of ϑ the space $X_{1+\vartheta}$ in general depends on t through the boundary condition $A(t)u = 0$ on $\partial\Omega$. Furthermore, under the above regularity assumptions on the coefficients of the differential operator $\mathcal{A}(x,t)$, the Hölder continuity of $A(t)$ on $X_{1+\vartheta}$ follows. As a consequence, the admissible value of ϑ in Hypothesis 2 is at most $1/4$.

These considerations also generalise to the Banach spaces $X = L^p(\Omega)$ with $D = W^{2,p}(\Omega) \cap W_0^{1,p}(\Omega)$, $1 < p < \infty$, see [5, Ex. 2].

In view of the numerical discretisation for (1.1), we introduce the following linear operators which are related to the analytic semigroup. For any sectorial operator $S : D \to X$ we set

$$\varphi(tS) = \frac{1}{t}\int_0^t \mathrm{e}^{(t-\tau)S}\,\mathrm{d}\tau, \qquad \psi(tS) = \frac{1}{t^2}\int_0^t \tau\mathrm{e}^{(t-\tau)S}\,\mathrm{d}\tau, \qquad t > 0. \tag{2.8a}$$

For later it is also essential that the relation

$$\psi(tS) - 1/2\,\varphi(tS) = tS\chi(tS) \tag{2.8b}$$

holds with a linear bounded operator $\chi(tS)$. Precisely, the estimate

$$\big\|t^{\nu-\mu}\varphi(tS)\big\|_{X_\nu\leftarrow X_\mu} + \big\|t^{\nu-\mu}\psi(tS)\big\|_{X_\nu\leftarrow X_\mu} + \big\|\chi(tS)\big\|_{X_\mu\leftarrow X_\mu} \le M \tag{2.8c}$$

is valid for $0 \le \mu \le \nu < 1$ and $t \in [0,T]$ with a constant $M > 0$. The bounds for $\varphi(tS)$ and $\psi(tS)$ are a direct consequence of the defining relations (2.8a) and (2.7), and the boundedness of $\chi(tS)$ follows by means of the integral formula of Cauchy.

3 Numerical method

In this section, we briefly discuss the concepts of Magnus integrators and exponential Runge–Kutta methods and then give a numerical scheme for (1.1).

Exponential and Magnus integration methods date back to the mid of the past century, we only mention the early works by Friedli [4], Lawson [17], and Magnus [19], and further refer to Minchev and Wright [20], where a historical survey is given. Both method classes require the numerical computation of the matrix exponential. This is a task that was considered as impracticable for many years, see Moler and Van Loan [21]. However, various recent works reflect the research activities on exponential and Magnus integrators, as a small selection of contributions concerned with the discretisation of stiff problems we mention [2, 11, 12, 13, 15, 16]. This renewed interest is explained by the fact that nowadays numerical methods are available which make it feasible to compute, in an efficient manner, matrix-vector products $\mathrm{e}^{tB}v$, see Hochbruck & Lubich [10] and references therein.

In the context of exponential Runge–Kutta methods, the basic idea for the numerical approximation of linear ordinary differential equations

$$y'(t) = Ay(t) + b(t), \qquad y(t_n) \text{ given},$$

is to represent the exact solution value at time $t_{n+1} = t_n + h$ by the variation-of-constants formula

$$y(t_{n+1}) = \mathrm{e}^{hA}y(t_n) + \int_0^h \mathrm{e}^{(h-\tau)A}b(t_n+\tau)\,\mathrm{d}\tau$$

and to replace the function $b(t_n + \tau)$ by a collocation polynomial through certain nodal points. In particular, for a single node at the midpoint this yields the following approximation $y_{n+1} \approx y(t_{n+1})$ by the *exponential midpoint rule*

$$y_{n+1} = \mathrm{e}^{hA}y_n + \int_0^h \mathrm{e}^{(h-\tau)A}\,\mathrm{d}\tau\, b\big(t_n + h/2\big), \tag{3.9}$$

which has classical order 2. A recent treatise of exponential integrators based on Runge–Kutta methods which includes a convergence analysis for parabolic problems is given in Hochbruck & Ostermann [12, 13].

On the other hand, for linear non-autonomous differential equations involving non-commuting matrices $A(t)$

$$y'(t) = A(t)y(t), \qquad y(t_n) \text{ given},$$

an approach studied by Magnus [19] is to write the exact solution in the form

$$y(t_n + s) = \mathrm{e}^{\Omega(s)} y(t_n),$$

where the time-dependent matrix Ω is given by the Magnus expansion, that is an infinite series involving iterated integrals of commutators of $A(t)$

$$\Omega(s) = \int_0^s A(t_n + \tau)\,\mathrm{d}\tau - \frac{1}{2}\int_0^s \Big[\int_0^\tau A(t_n+\sigma)\,\mathrm{d}\sigma, A(t_n+\tau)\Big]\,\mathrm{d}\tau + \cdots .$$

For the numerical approximation the expansion is truncated and the integrals are calculated by means of a quadrature formula, see for instance [2, 14, 29] in the context of geometric integration and Schrödinger equations, respectively. By truncating the Magnus expansion after the first term and applying the midpoint rule in order to approximate the integral, we receive the following recursion for the numerical solution

$$y_{n+1} = \mathrm{e}^{hA(t_n+h/2)} y_n. \tag{3.10}$$

Concerning the error behaviour of this Magnus integrator applied to stiff equations, the following results are known. In Hochbruck & Lubich [11] a second-order error estimate is derived for spatial discretisations of time-dependent Schrödinger type equations. For abstract parabolic problems it is shown in [5] that the Magnus integrator is convergent of order 2 in the underlying function space. However, if the error is measured in the domain of the differential operator, an order reduction occurs, in general.

The above considerations and the numerical scheme given in [5] motivate the following numerical method for differential equations of the form (1.1). Henceforth, for a constant stepsize $h > 0$ we denote by $t_n = nh$ the associated grid points and further set $t_{n+1/2} = t_n + h/2$ for $n \geq 0$. Combining the second-order Magnus integrator (3.10) and the exponential midpoint rule (3.9) yields the recursion

$$u_{n+1} = \mathrm{e}^{hA(t_{n+1/2})} u_n + \int_0^h \mathrm{e}^{(h-\tau)A(t_{n+1/2})}\,\mathrm{d}\tau\, b\big(t_{n+1/2}, u_{n+1/2}\big)$$

for u_{n+1} approximating the exact solution value at time t_{n+1}. Here, the additional internal stage $u_{n+1/2} \approx u(t_{n+1/2})$ is determined through the first-order formula

$$u_{n+1/2} = \mathrm{e}^{h/2\,A(t_{n+1/2})} u_n + \int_0^{h/2} \mathrm{e}^{(h/2-\tau)A(t_{n+1/2})}\,\mathrm{d}\tau\, b(t_n, u_n).$$

From (2.7b) applied with $\vartheta = \beta$ it follows at once that $u_{n+1/2}$ and thus u_{n+1} lies in X_β whenever u_n is chosen in X_β, provided that the function b is bounded in X. With the help of the abbreviations

$$A_{n+1/2} = A\big(t_{n+1/2}\big), \quad b_n = b(t_n, u_n), \quad b_{n+1/2} = b\big(t_{n+1/2}, u_{n+1/2}\big), \tag{3.11a}$$

the numerical scheme can be written as

$$\begin{aligned} u_{n+1/2} &= \mathrm{e}^{h/2\, A_{n+1/2}} u_n + h/2\, \varphi\big(h/2\, A_{n+1/2}\big)\, b_n, \\ u_{n+1} &= \mathrm{e}^{hA_{n+1/2}} u_n + h\, \varphi\big(hA_{n+1/2}\big)\, b_{n+1/2}, \qquad n \geq 0, \end{aligned} \tag{3.11b}$$

see also (2.8a). By Taylor series expansions it is straightforward to show that this method has classical order 2.

As the nonlinear part is integrated explicitely, the scheme (3.11) resembles a linearly-explicit Runge–Kutta method, see Strehmel and Weiner [25, Ch. 4]. However, utilising exponentials instead of rational functions enhances the stability properties of the integrator. We further remark that (3.11) can also be considered as a Runge–Kutta Munthe–Kaas method, see Munthe–Kaas [22].

Concerning the realisation of (3.11) by means of Krylov subspace methods, it is useful to note that the analytic semigroup and the closely related operator φ satisfy the relations

$$\begin{aligned} \mathrm{e}^{hA_{n+1/2}} &= \mathrm{e}^{h/2\, A_{n+1/2}}\, \mathrm{e}^{h/2\, A_{n+1/2}}, \\ \varphi\big(hA_{n+1/2}\big) &= 1/2\, \big(I + \mathrm{e}^{h/2\, A_{n+1/2}}\big) \varphi\big(h/2\, A_{n+1/2}\big). \end{aligned}$$

Thus, it is desirable to make use of the information obtained from the computation of the internal stage $u_{n+1/2}$ such that only a small amount of additional work is required for the computation of the numerical solution u_{n+1}. We are not aware that this numerical linear algebra task has been resolved yet.

For abstract linear parabolic problems (1.2), the numerical scheme (3.11) simplifies as follows

$$u_{n+1} = \mathrm{e}^{hA_{n+1/2}} u_n + h\, \varphi\big(hA_{n+1/2}\big)\, b\big(t_{n+1/2}\big), \qquad n \geq 0. \tag{3.12}$$

In our previous work [5], employing Hypotheses 1-2 with $\vartheta = 0$ and the temporal smoothness of A and b, we proved a second order error estimate for (3.12) in the norm of the underlying function space X. The main objective of the present work is to extend the convergence analysis of [5] to semilinear parabolic problems. It is interesting to note that in the present situation, for smooth initial values $u_0 \in X_\beta$, it follows at once that the numerical approximation (3.11) remains well-defined in X_β, whereas the existence of the exact solution of (1.1) has to be established by Banach's Fixed-point Theorem, see also [18]. Concerning the techniques applied in this paper, the main differences to linear equations are the following. Due to the presence of an additional internal stage, the derivation of a suitable expansion for the global error is more involved, see Section 5.1. Further, as the flow of the equation belongs to the domain of the nonlinearity, it is natural to measure also the error in the intermediate space X_β. In the subsequent Section 4, we derive stability bounds with respect to the norm of certain intermediate spaces. These auxiliary estimates are needed in Section 5.2 for proving the convergence result.

4 Stability bounds

In this section, we study the stability properties of (3.11) when applied to the homogeneous problem

$$u'(t) = A(t)u(t), \quad 0 < t \leq T, \qquad u(0) = u_0. \tag{4.13}$$

In this case, the numerical approximation is given by

$$u_{n+1} = \mathrm{e}^{hA_{n+1/2}} u_n = \mathrm{e}^{hA_{n+1/2}} \mathrm{e}^{hA_{n-1/2}} \cdots \mathrm{e}^{hA_{1/2}} u_0, \qquad n \geq 0.$$

We recall the abbreviation $A_{i+1/2} = A(t_{i+1/2})$ where $t_{i+1/2} = t_i + h/2$. In Theorem 1 below, we state a stability estimate for the discrete evolution operator

$$E_m^n = \mathrm{e}^{hA_{n+1/2}} \mathrm{e}^{hA_{n-1/2}} \cdots \mathrm{e}^{hA_{m+1/2}}, \qquad n > m \geq 0, \tag{4.14}$$

and further specify a refined bound which is needed in the proof of Theorem 2. The corresponding estimates for the analytic semigroup generated by the sectorial operator $A_{m+1/2}$ are

$$\begin{aligned} \big\| \mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}} \big\|_{X_\nu \leftarrow X_\mu} &\leq M (t_{n+1} - t_m)^{-\nu+\mu}, \\ \big\| A_{m+1/2}\, \mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}} \chi\big(hA_{m+1/2}\big) \big\|_{X_\nu \leftarrow X_\mu} &\leq M (t_{n+1} - t_m)^{-1-\nu+\mu}, \end{aligned} \tag{4.15}$$

where $0 \leq \mu \leq \nu < 1$ and $0 \leq t_m \leq t_n \leq T$, see (2.7) and (2.8).

Theorem 1 *Under Hypotheses 1-2 with $\vartheta = \mu$ the estimate*

$$\big\| E_m^n \big\|_{X_\nu \leftarrow X_\mu} \leq C (t_{n+1} - t_m)^{-\nu+\mu}, \qquad 0 \leq t_m < t_n \leq T, \tag{4.16a}$$

is valid for $0 \leq \mu \leq \nu < 1$ with constant $C > 0$ not depending on n and h. Moreover, provided that Hypothesis 2 holds with $\alpha = 1$, the bound

$$\begin{aligned} \big\| E_m^n A_{m+1/2}\, \chi\big(hA_{m+1/2}\big) \big\|_{X_\nu \leftarrow X_\mu} &\leq C (t_{n+1} - t_m)^{-1-\nu+\mu} \\ &\quad + C \big(1 + |\log h|\big) (t_{n+1} - t_m)^{-\nu+\mu} \end{aligned} \tag{4.16b}$$

follows.

Proof. As the techniques for deriving the stability bounds in (4.16) are close to that applied in [5], we only sketch the main steps of the proof.

Comparing the discrete evolution operator E_m^n with the analytic semigroup $\mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}}$, we employ a telescopic identity for the difference

$$\begin{aligned} \Delta_m^n &= E_m^n - \mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}} \\ &= \sum_{j=m+1}^{n-1} \Delta_{j+1}^n \big(\mathrm{e}^{hA_{j+1/2}} - \mathrm{e}^{hA_{m+1/2}}\big) \mathrm{e}^{(t_j - t_m)A_{m+1/2}} \\ &\quad + \sum_{j=m+1}^{n} \mathrm{e}^{(t_{n+1}-t_{j+1})A_{m+1/2}} \big(\mathrm{e}^{hA_{j+1/2}} - \mathrm{e}^{hA_{m+1/2}}\big) \mathrm{e}^{(t_j - t_m)A_{m+1/2}}. \end{aligned} \tag{4.17}$$

By means of the integral formula of Cauchy, the operator

$$\Xi_{jm} = \big(\mathrm{e}^{hA_{j+1/2}} - \mathrm{e}^{hA_{m+1/2}}\big) \mathrm{e}^{(t_j - t_m)A_{m+1/2}}, \qquad j > m,$$

is represented through a path integral

$$\begin{aligned} \Xi_{jm} = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^\lambda \big(\lambda I - hA_{j+1/2}\big)^{-1} h \big(A_{j+1/2} - A_{m+1/2}\big) \\ \times \big(\lambda I - hA_{m+1/2}\big)^{-1} \mathrm{e}^{(t_j - t_m)A_{m+1/2}}\, \mathrm{d}\lambda, \end{aligned}$$

where Γ is chosen in such a way that it surrounds the spectrum of the sectorial operators $A_{j+1/2}$ and $A_{m+1/2}$, see also (2.6). The main tools for estimating Ξ_{jm} are the resolvent bound (2.3) as well as the corresponding relations on the intermediate spaces. Further, we apply the bounds (2.7) for the analytic semigroup and the Hölder-estimate of Hypothesis 2 with $\vartheta = \mu$. As a consequence, we receive

$$\big\|\Xi_{jm}\big\|_{X_\mu \leftarrow X_\mu} \le Ch(t_j - t_m)^{-1+\alpha}, \qquad \big\|\Xi_{jm}\big\|_{X_\nu \leftarrow X_\mu} \le Ch^{1-\nu+\mu}(t_j - t_m)^{-1+\alpha}.$$

With the help of these relations, we estimate Δ_m^n as operator from X_μ to X_ν

$$\begin{aligned}
\big\|\Delta_m^n\big\|_{X_\nu \leftarrow X_\mu} &\le \sum_{j=m+1}^{n-1} \big\|\Delta_{j+1}^n\big\|_{X_\nu \leftarrow X_\mu} \big\|\Xi_{jm}\big\|_{X_\mu \leftarrow X_\mu} + \big\|\Xi_{nm}\big\|_{X_\nu \leftarrow X_\mu} \\
&\quad + \sum_{j=m+1}^{n-1} \big\|\mathrm{e}^{(t_{n+1}-t_{j+1})A_{m+1/2}}\big\|_{X_\nu \leftarrow X_\mu} \big\|\Xi_{jm}\big\|_{X_\mu \leftarrow X_\mu} \\
&\le Ch \sum_{j=m+1}^{n-1} \big\|\Delta_{j+1}^n\big\|_{X_\nu \leftarrow X_\mu} (t_j - t_m)^{-1+\alpha} \\
&\quad + Ch \sum_{j=m+1}^{n-1} (t_{n+1} - t_{j+1})^{-\nu+\mu} (t_j - t_m)^{-1+\alpha}.
\end{aligned}$$

We interprete the second sum as a Riemann-sum and bound it by the associated integral. From a Gronwall-type inequality with a weakly singular kernel, see [3, 23], we further obtain

$$\big\|\Delta_m^n\big\|_{X_\nu \leftarrow X_\mu} \le C(t_{n+1} - t_m)^{-\nu+\mu+\alpha}. \tag{4.18}$$

Thus, together with (4.15) the first bound in (4.16) follows.

For proving (4.16b), as before, we correlate the discrete evolution operator with the analytic semigroup generated by $A_{m+1/2}$. From the above relation (4.17), by employing the abbreviation

$$\widetilde{\Xi}_{jm} = \big(\mathrm{e}^{hA_{j+1/2}} - \mathrm{e}^{hA_{m+1/2}}\big) A_{m+1/2}\, \mathrm{e}^{(t_j-t_m)A_{m+1/2}} \chi\big(hA_{m+1/2}\big), \qquad j > m,$$

we receive the following identity

$$\begin{aligned}
&E_m^n A_{m+1/2} \chi\big(hA_{m+1/2}\big) \\
&\quad = \Delta_m^n A_{m+1/2}\, \chi\big(hA_{m+1/2}\big) + A_{m+1/2}\, \mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}}\, \chi\big(hA_{m+1/2}\big) \\
&\quad = \sum_{j=m+1}^{n-1} \Delta_{j+1}^n\, \widetilde{\Xi}_{jm} + \sum_{j=m+1}^{n} \mathrm{e}^{(t_{n+1}-t_{j+1})A_{m+1/2}}\, \widetilde{\Xi}_{jm} \\
&\qquad + A_{m+1/2}\, \mathrm{e}^{(t_{n+1}-t_m)A_{m+1/2}}\, \chi\big(hA_{m+1/2}\big).
\end{aligned} \tag{4.19}$$

Under Hypothesis 2 with $\alpha = 1$ it holds

$$\big\|\widetilde{\Xi}_{jm}\big\|_{X_\mu \leftarrow X_\mu} \le Ch(t_j - t_m)^{-1}, \qquad \big\|\widetilde{\Xi}_{jm}\big\|_{X_\nu \leftarrow X_\mu} \le Ch^{1-\nu+\mu}(t_j - t_m)^{-1}.$$

Therefore, an estimation of (4.19) by means of (4.15) and (4.18) finally yields the desired result. $\square$

5 Convergence

The present section is devoted to the derivation of a convergence result for the numerical method (3.11) applied to the abstract initial value problem (1.1). The error estimate with respect to the norm of the domain of the nonlinearity is stated in Section 5.2 below. The proof of Theorem 2 is based on a suitable representation of the global error which we derive next.

5.1 Relation for error

For the subsequent considerations, it is convenient to introduce several short notations. Recall the abbreviations $t_{n+1/2} = t_n + h/2 = nh + h/2$, $A_{n+1/2} = A\big(t_{n+1/2}\big)$, $b_n = b(t_n, u_n)$, and $b_{n+1/2} = b\big(t_{n+1/2}, u_{n+1/2}\big)$, introduced before in Section 3. Also, we set $A_n = A(t_n)$. The values of the exact solution are denoted by

$$\widehat{u}_n = u(t_n), \quad \widehat{u}_{n+1/2} = u\big(t_{n+1/2}\big), \quad \widehat{b}_n = b\big(t_n, \widehat{u}_n\big), \quad \widehat{b}_{n+1/2} = b\big(t_{n+1/2}, \widehat{u}_{n+1/2}\big).$$

Then, the following quantities

$$e_n = u_n - \widehat{u}_n, \qquad e_{n+1/2} = u_{n+1/2} - \widehat{u}_{n+1/2},$$

signify the global error of the numerical approximation and the internal stage, respectively.

For representing the error e_{n+1} in a suitable manner, we consider the relation for the numerical approximation u_{n+1} in (3.11) and derive a similar formula for the exact solution value $\widehat{u}_{n+1}$. Rewriting the right-hand side of the equation (1.1) by adding and substracting $A_{n+1/2}$ and $b_{n+1/2}$ gives

$$u'(t) = A(t)u(t) + b\big(t, u(t)\big) = A_{n+1/2}\, u(t) + b_{n+1/2} + R_n(t),$$

where the map $R_n : [t_n, t_{n+1}] \to X$ comprises the remaining terms

$$R_n(t) = \big(A(t) - A_{n+1/2}\big)u(t) + b\big(t, u(t)\big) - b_{n+1/2}. \tag{5.20}$$

By the variation-of-constants formula and (2.8a), we therefore receive

$$\widehat{u}_{n+1} = \mathrm{e}^{hA_{n+1/2}}\widehat{u}_n + h\,\varphi\big(hA_{n+1/2}\big)\, b_{n+1/2} + D_{n+1}, \tag{5.21}$$

with D_{n+1} denoting the defect of the method

$$D_{n+1} = \int_0^h \mathrm{e}^{(h-\tau)A_{n+1/2}} R_n(t_n + \tau)\,\mathrm{d}\tau. \tag{5.22}$$

Taking the difference of (3.11) and (5.21) yields

$$e_{n+1} = \mathrm{e}^{hA_{n+1/2}}\, e_n - D_{n+1}, \qquad e_0 = 0.$$

By resolving this error recursion, we finally obtain the following relation for e_n involving the discrete evolution operator defined through (4.14)

$$e_n = -\sum_{j=0}^{n-1} E_{j+1}^{n-1} D_{j+1}. \tag{5.23}$$

In order to represent the defects in a suitable way, we write the remainder R_n given by (5.20) in the form

$$R_n(t) = r_n(t) + \widehat{b}_{n+1/2} - b_{n+1/2}. \tag{5.24a}$$

Provided that $b(t,v)$ is differentiable with respect to the second variable v, we have

$$\widehat{b}_{n+1/2} - b_{n+1/2} = -\, B_{n+1/2}\, e_{n+1/2}, \tag{5.24b}$$

with $B_{n+1/2}$ denoting the integral

$$B_{n+1/2} = \int_0^1 D_v b\big(t_{n+1/2}, \sigma\, \widehat{u}_{n+1/2} + (1-\sigma) u_{n+1/2}\big)\, \mathrm{d}\sigma. \tag{5.24c}$$

Furthermore, under the assumption that the map

$$r_n(t) = \big(A(t) - A_{n+1/2}\big) u(t) + b\big(t, u(t)\big) - \widehat{b}_{n+1/2} \tag{5.24d}$$

is twice differentiable on (t_n, t_{n+1}), we obtain from a Taylor series expansion the following identity

$$\begin{aligned} r_n(t_n+\tau) &= \big(\tau - h/2\big)\, r_n'\big(t_{n+1/2}\big) \\ &\quad + \big(\tau - h/2\big)^2 \int_0^1 (1-\sigma)\, r_n''\big(t_{n+1/2} + \sigma\big(\tau - h/2\big)\big)\, \mathrm{d}\sigma, \end{aligned} \tag{5.24e}$$

where $\tau \in (0,h)$. According to (5.22), we determine D_{n+1} with the help of the above relations (5.24) and (2.8a)-(2.8b). Altogether, we receive the representation

$$D_{n+1} = d_{n+1} + \delta_{n+1}, \tag{5.25a}$$

where $d_{n+1} = d_{n+1}^{(0)} + d_{n+1}^{(1)}$ comprises the terms

$$\begin{aligned} d_{n+1}^{(0)} &= h^2 \big(\psi\big(hA_{n+1/2}\big) - 1/2\, \varphi\big(hA_{n+1/2}\big)\big)\, r_n'\big(t_{n+1/2}\big) \\ &= h^3 A_{n+1/2}\, \chi\big(hA_{n+1/2}\big)\, r_n'\big(t_{n+1/2}\big), \\ d_{n+1}^{(1)} &= \int_0^h \mathrm{e}^{(h-\tau)A_{n+1/2}} \big(\tau - h/2\big)^2 \int_0^1 (1-\sigma)\, r_n''\big(t_{n+1/2} + \sigma\big(\tau - h/2\big)\big)\, \mathrm{d}\sigma\, \mathrm{d}\tau. \end{aligned} \tag{5.25b}$$

Further, the defect δ_{n+1} is given by

$$\delta_{n+1} = -\, h\, \varphi\big(hA_{n+1/2}\big)\, B_{n+1/2}\, e_{n+1/2}. \tag{5.25c}$$

As δ_{n+1} involves the error of the internal stage, it remains to derive a suitable relation for $e_{n+1/2}$. Similar to before, we consider the equation (1.1) on the interval $[t_n, t_{n+1}]$ and rewrite the right-hand side as follows

$$u'(t) = A_{n+1/2} u(t) + b_n + S_n(t), \qquad S_n(t) = \big(A(t) - A_{n+1/2}\big) u(t) + b\big(t, u(t)\big) - b_n.$$

Thus, an application of the variation-of-constants formula yields

$$\widehat{u}_{n+1/2} = \mathrm{e}^{h/2\, A_{n+1/2}} \widehat{u}_n + h/2\, \varphi\big(h/2\, A_{n+1/2}\big)\, b_n + \Theta_{n+1},$$

with defect Θ_{n+1} given by

$$\Theta_{n+1} = \int_0^{h/2} \mathrm{e}^{(h/2-\tau)A_{n+1/2}} S_n(t_n+\tau)\,\mathrm{d}\tau.$$

As a consequence, together with the first formula in (3.11), we have

$$e_{n+1/2} = \mathrm{e}^{h/2\,A_{n+1/2}}\, e_n - \Theta_{n+1}. \tag{5.26}$$

In order to represent Θ_{n+1} in a favourable way, we write the remainder S_n in the form

$$S_n(t) = s_n(t) + \big(A_n - A_{n+1/2}\big)u(t) + \widehat{b}_n - b_n,$$

where $s_n : [t_n, t_{n+1}] \to X$ is defined through

$$s_n(t) = \big(A(t) - A_n\big)u(t) + b\big(t, u(t)\big) - \widehat{b}_n. \tag{5.27}$$

Again, we receive from Taylor series expansions of $s_n(t_n+\tau)$, $A_n - A_{n+1/2}$, and $\widehat{b}_n - b_n$ and from a succeeding integration the relation

$$\Theta_{n+1} = \theta_{n+1} + \eta_{n+1}. \tag{5.28a}$$

Here, θ_{n+1} is further decomposed into $\theta_{n+1} = \theta^{(0)}_{n+1} + \theta^{(1)}_{n+1} + \theta^{(2)}_{n+1}$ with

$$\begin{aligned}
\theta^{(0)}_{n+1} &= h^2/4\,\psi\big(h/2\,A_{n+1/2}\big)\, s_n'(t_n),\\
\theta^{(1)}_{n+1} &= \int_0^{h/2} \mathrm{e}^{(h/2-\tau)A_{n+1/2}}\,\tau^2 \int_0^1 (1-\sigma)\, s_n''(t_n+\sigma\tau)\,\mathrm{d}\sigma\,\mathrm{d}\tau,\\
\theta^{(2)}_{n+1} &= -\,h/2 \int_0^{h/2} \mathrm{e}^{(h/2-\tau)A_{n+1/2}} \int_0^1 A'\big(t_n + (1-\sigma)h/2\big)\,\mathrm{d}\sigma\, u(t_n+\tau)\,\mathrm{d}\tau,
\end{aligned} \tag{5.28b}$$

and the second term η_{n+1} equals

$$\eta_{n+1} = -\,h/2\,\varphi\big(h/2\,A_{n+1/2}\big)B_n e_n, \qquad B_n = \int_0^1 D_v b\big(t_n, \sigma\,\widehat{u}_n + (1-\sigma)u_n\big)\,\mathrm{d}\sigma. \tag{5.28c}$$

Consequently, by applying successively the relations (5.25), (5.26), and (5.28), we receive

$$\begin{aligned}
D_{n+1} = d_{n+1} &- h\,\varphi\big(hA_{n+1/2}\big)\, B_{n+1/2}\\
&\times \big(\mathrm{e}^{h/2\,A_{n+1/2}}\, e_n - \theta_{n+1} + h/2\,\varphi\big(h/2\,A_{n+1/2}\big)B_n e_n\big).
\end{aligned}$$

Finally, we insert this identity into the error recursion (5.23) and obtain the following representation for the global error $e_n = e_n^{(0)} + e_n^{(1)} + e_n^{(2)}$, where

$$\begin{aligned}
e_n^{(0)} &= h \sum_{j=0}^{n-1} E_{j+1}^{n-1} \varphi\big(hA_{j+1/2}\big) B_{j+1/2}\big(\mathrm{e}^{h/2\,A_{j+1/2}} + h/2\,\varphi\big(h/2\,A_{j+1/2}\big)B_j\big)e_j,\\
e_n^{(1)} &= -\sum_{j=0}^{n-1} E_{j+1}^{n-1} d_{j+1}, \qquad e_n^{(2)} = -h \sum_{j=0}^{n-1} E_{j+1}^{n-1} \varphi\big(hA_{j+1/2}\big) B_{j+1/2}\,\theta_{j+1},
\end{aligned} \tag{5.29}$$

with defects $d_{n+1} = d^{(0)}_{n+1} + d^{(1)}_{n+1}$ and $\theta_{n+1} = \theta^{(0)}_{n+1} + \theta^{(1)}_{n+1} + \theta^{(2)}_{n+1}$ given by (5.25b) and (5.28b).

5.2 Error estimate

In this section, we prove a convergence estimate for the numerical discretisation (3.11) of the semilinear parabolic problem (1.1) with respect to the norm of the domain of the nonlinearity. The main tools for the derivation of this error bound are the representation (5.29) for the global error and the stability estimates for the discrete evolution operator stated in Section 4. In view of Theorem 2, for any map $g_n : [t_n, t_{n+1}] \to X$ defined for integers $n \geq 0$ we henceforth set

$$\|g\|_{X,\infty} = \max_{0\leq j\leq n-1} \|g_j\|_{X,\infty}, \qquad \text{where} \quad \|g_j\|_{X,\infty} = \max_{t_j\leq t\leq t_{j+1}} \big\|g_j(t)\big\|_X.$$

We note that the differentiability of the functions r_n and s_n introduced in (5.24d) and (5.27) is governed by the smoothness of the exact solution u and the data A and b. In particular, in the situation of the theorem, Hypothesis 2 is always fulfilled with $\alpha = 1$. Also, the requirement that the first derivatives of r_n and s_n are bounded in some intermediate space X_γ is in general satisfied in applications for sufficiently small values of $\gamma > 0$, see Example 1 and the discussion in Section 6.

Theorem 2 (Convergence) *Suppose that Hypotheses 1-3 are fulfilled with $\alpha = 1$ and $\vartheta = \gamma$ for $0 \leq \gamma \leq \beta < 1$. Then, the numerical method* (3.11) *applied to the abstract initial value problem* (1.1) *satisfies the convergence estimate*

$$\begin{aligned}\big\|u_n - u(t_n)\big\|_{X_\beta} &\leq Ch^{2-\beta+\gamma}\Big(\big(1+|\log h|\big)\|r'\|_{X_\gamma,\infty} + \big\|s'\big\|_{X_\gamma,\infty}\Big)\\ &\quad + Ch^2\Big(\big\|r''\big\|_{X,\infty} + Ch^2\big\|s''\big\|_{X,\infty}\Big), \qquad 0 \leq t_n \leq T,\end{aligned}$$

provided that the quantities on the right-hand side are well-defined. The constant $C > 0$ does not depend on n and h.

Remark 1 In the present work, for notational simplicity, we suppose $u_0 = u(0)$. If the numerical initial value u_0 is different from the true initial value $u(0)$, the statement of Theorem 2 remains valid with an additional term $C\big\|u_0 - u(0)\big\|_{X_\beta}$ in the error estimate, provided that u_0 and $u(0)$ belong to X_β.

Proof of Theorem 2. In the sequel, we estimate the global error in the norm of the intermediate space X_β. For that purpose, we successively consider the error terms in (5.29) which we estimate with the help of the stability bounds from Theorem 1 and the bounds for the analytic semigroup and the related operators, see (2.7) and (2.8c). Note that $E_{j+1}^{n-1} = I$ for $j = n-1$.

On the one hand, a direct estimation of $e_n^{(0)}$ yields

$$\big\|e_n^{(0)}\big\|_{X_\beta} \leq Ch\sum_{j=0}^{n-2}(t_n - t_{j+1})^{-\beta}\|e_j\|_{X_\beta} + Ch^{1-\beta}\|e_{n-1}\|_{X_\beta}.$$

By inserting formula (5.25b) for $d_{n+1} = d_{n+1}^{(0)} + d_{n+1}^{(1)}$ into (5.29), it follows

$$\begin{aligned}\big\|e_n^{(1)}\big\|_{X_\beta} &\leq h^3\sum_{j=0}^{n-2}\big\|E_{j+1}^{n-1}A_{j+1/2}\,\chi\big(hA_{j+1/2}\big)\big\|_{X_\beta\leftarrow X_\gamma}\big\|r_j'\big(t_{j+1/2}\big)\big\|_{X_\gamma}\\ &\quad + h^2\Big(\big\|\psi\big(hA_{n-1/2}\big)\big\|_{X_\beta\leftarrow X_\gamma} + 1/2\,\big\|\varphi\big(hA_{n-1/2}\big)\big\|_{X_\beta\leftarrow X_\gamma}\Big)\\ &\qquad \times\big\|r_{n-1}'\big(t_{n-1/2}\big)\big\|_{X_\gamma} + \sum_{j=0}^{n-2}\big\|E_{j+1}^{n-1}\big\|_{X_\beta\leftarrow X}\big\|d_{j+1}^{(1)}\big\|_X + \big\|d_n^{(1)}\big\|_{X_\beta}\end{aligned}$$

and therefore

$$\big\|e_n^{(1)}\big\|_{X_\beta} \le Ch^{2-\beta+\gamma}\big(1+|\log h|\big)\big\|r'\big\|_{X_\gamma,\infty} + Ch^2\big\|r''\big\|_{X,\infty}.$$

Furthermore, by means of relation (5.28b) for the defect $\theta_{n+1} = \theta_{n+1}^{(0)} + \theta_{n+1}^{(1)} + \theta_{n+1}^{(2)}$, we obtain the following bound for the remaining term $e_n^{(2)}$

$$\big\|e_n^{(2)}\big\|_{X_\beta} \le Ch^{2-\beta+\gamma}\big(\big\|A'u\big\|_{X_\gamma,\infty} + \big\|s'\big\|_{X_\gamma,\infty}\big) + Ch^2\big\|s''\big\|_{X,\infty}.$$

Here, we employ the abbreviation $\|A'u\|_{X_\gamma,\infty}$ for the maximum value of the map $A'\big(t_j+(1-\sigma)h/2\big)u(t_j+\tau)$ in X_γ over all values of $0 \le \sigma, \tau/h \le 1$ and $0 \le j \le n-1$. Now, from a Gronwall inequality, the desired error estimate follows. For notational simplicity, in the statement of the theorem we omit the term involving $A'u$ as it is in general dominated by the first derivatives of r and s. □

Remark 2 Going over the proofs of Theorem 1 and Theorem 2 shows that the employed techniques are not restricted to constant stepsizes and extend to variable stepsizes where the ratios are bounded from below and above by (moderate) constants $C_1 \le h_j/h_{j-1} \le C_2$. We do not elaborate this point here and refer to [27], where similar investigations have been carried out for variable stepsize linear multistep methods.

We conclude this section with a remark on the stability of the considered numerical scheme. For that purpose, we define sequences $(v_n)_{n\ge 0}$ and $(w_n)_{n\ge 0}$ accordingly to (3.11), assuming $v_0, w_0 \in X_\beta$. A Taylor series expansion implies the following relation for the difference $z_n = v_n - w_n$

$$\begin{aligned} z_{n+1/2} &= \mathrm{e}^{h/2\,A_{n+1/2}} z_n + h/2\,\varphi\big(h/2\,A_{n+1/2}\big)\,\widetilde{B}_n\, z_n, \\ z_{n+1} &= \mathrm{e}^{hA_{n+1/2}} z_n + h\,\varphi\big(hA_{n+1/2}\big)\,\widetilde{B}_{n+1/2}\, z_{n+1/2}, \qquad n \ge 0. \end{aligned}$$

Here, we employ the abbreviations

$$\begin{aligned} \widetilde{B}_n &= \int_0^1 D_v b\big(t_n, \sigma\, v_n + (1-\sigma)w_n\big)\,\mathrm{d}\sigma, \\ \widetilde{B}_{n+1/2} &= \int_0^1 D_v b\big(t_{n+1/2}, \sigma\, v_{n+1/2} + (1-\sigma)w_{n+1/2}\big)\,\mathrm{d}\sigma. \end{aligned}$$

Furthermore, we receive

$$\begin{aligned} z_n = E_0^{n-1} z_0 + h \sum_{j=0}^{n-1} & E_{j+1}^{n-1}\varphi\big(hA_{j+1/2}\big)\widetilde{B}_{j+1/2} \\ & \times \Big(\mathrm{e}^{h/2\,A_{j+1/2}} + h/2\,\varphi\big(h/2\,A_{j+1/2}\big)\widetilde{B}_j\Big) z_j, \qquad n \ge 0, \end{aligned}$$

see Section 5.1. Under Hypotheses 1-3 with $\vartheta = 0$, making use of the stability bounds for the discrete evolution operator provided by Theorem 1, it follows

$$\|v_n - w_n\|_{X_\beta} \le C\|v_0 - w_0\|_{X_\beta}, \qquad n \ge 0.$$

We omit the details and refer to the proof of Theorem 2, where similar arguments are employed.

h\M	200	300	400	500	600	700	800	900
2^{-3}	1.7988	1.7987	1.7987	1.7987	1.7987	1.7987	1.7987	1.7987
2^{-4}	1.7504	1.7503	1.7503	1.7502	1.7502	1.7502	1.7502	1.7502
2^{-5}	1.7499	1.7497	1.7496	1.7496	1.7496	1.7496	1.7496	1.7496
2^{-6}	1.7498	1.7495	1.7493	1.7493	1.7493	1.7492	1.7492	1.7492
2^{-7}	1.7503	1.7496	1.7494	1.7492	1.7492	1.7491	1.7491	1.7491
2^{-8}	1.7516	1.7502	1.7497	1.7495	1.7494	1.7493	1.7493	1.7493
2^{-9}	1.7541	1.7515	1.7505	1.7501	1.7498	1.7497	1.7496	1.7495
2^{-10}	1.7591	1.7538	1.7519	1.7510	1.7505	1.7502	1.7501	1.7499

Table 1: Numerically observed temporal convergence order in a discrete H^1_0-norm for discretisations with spatial grid length $\Delta x = (M+1)^{-1}$ and time-step h.

6 Numerical example

In order to illustrate the convergence result, we consider a one-dimensional initial-boundary value problem comprising the following partial differential equation for a function $U : [0,1] \times [0,1] \to \mathbb{R}$

$$\partial_t U(x,t) = \alpha(x,t)\partial_{xx}U(x,t) + \beta(x,t)U(x,t)\,\partial_x U(x,t) + g\big(x,t,U(x,t)\big), \quad (6.30a)$$

subject to a homogeneous Dirichlet boundary condition and an initial condition

$$U(0,t) = 0 = U(1,t), \quad 0 \le t \le 1, \qquad U(x,0) = U_0(x), \quad 0 \le x \le 1. \quad (6.30b)$$

Under certain regularity and boundedness requirements on the coefficients α and β and on the function g, by setting

$$\big(A(t)v\big)(x) = \mathcal{A}(x,t)v(x) = \alpha(x,t)\,\partial_{xx}v(x),$$
$$b(t,v)(x) = f\big(x,t,v(x),\partial_x v(x)\big) = \beta(x,t)v(x)\,\partial_x v(x) + g\big(x,t,v(x)\big),$$

we conclude from the previous Example 1 that this problem can be cast into the abstract framework for

$$X = L^2(0,1), \qquad D = H^2(0,1) \cap H^1_0(0,1), \qquad X_\beta = X_{1/2} = H^1_0(0,1).$$

Provided that α, β, and g are sufficiently smooth in space and time, but do not satisfy additional boundary conditions, it follows that the admissible values of γ in Theorem 2 are $0 \le \gamma < 1/4$. Thus, the expected fractional convergence order with respect to the norm of the Sobolev space $X_\beta = H^1_0(0,1)$ is

$$\kappa = 2 - \beta + \gamma, \qquad \beta = 1/2, \qquad \gamma < 1/4. \quad (6.31)$$

We note that it is straightforward to extend the above considerations to an initial value problem obtained from a finite difference spatial discretisation of (6.30).

For the numerical experiment, in order to keep the implementation simple, we choose $\alpha(x,t) = 1 + \mathrm{e}^{-t}$ and $\beta(x,t) = -1$ and determine the function g and the initial condition U_0 such that the exact solution of the initial-boundary value problem (6.30) is given by $U(x,t) = x(1-x)\,\mathrm{e}^{-t}$. In particular, the exact solution belongs to the domain D. Further, the coefficients α and β and the map g fulfill the required regularity and boundedness conditions, see also Henry [9, Sect. 3.3].

The partial differential equation is discretised in space by symmetric finite differences of grid length $\Delta x = (M+1)^{-1}$. Due to the special choice of the exact solution, the spatial discretisation error is zero. In order to solve the resulting system of ordinary differential equations, we apply the numerical method (3.11). As the coefficient α does not depend on the space variable x, for the spatially discretised system the required matrix exponentials are calculated rapidly by Fourier techniques. We mention that in more general situations where spectral techniques are not applicable, an alternative implementation of the exponential and the related φ-function is provided by a recently developed MATLAB package, see [1]. The numerical temporal order of convergence with respect to a discrete H_0^1-norm is determined from the numerical and exact solution values. The obtained numbers are displayed in Table 1. The values of approximately 1.75 are in accordance with the convergence order (6.31) predicted by Theorem 2.

7 Concluding remarks

In the present paper, proceeding our previous work [5] on linear parabolic problems, we study the convergence properties of a Magnus type integrator for semilinear problems. Provided that the efficient calculation of the matrix exponential and the related φ-function is feasible, the considered numerical scheme has the following benefits. It is explicit in the nonlinearity and possesses favourable stability and convergence properties for stiff problems at a reasonable computational effort.

The given error analysis is primarily of theoretical value and gives insight how to construct and study an explicit exponential integration scheme for quasilinear parabolic problems, which are relevant for practical applications, see [6]. For instance, such problems arise in the modelling of diffusion processes with state-dependent diffusivity and in the study of fluids in porous media.

Concerning the derivation of Magnus type integrators of higher order, up to now, the following approaches were studied. In [28], the error behaviour of a fourth-order commutator-free exponential integrator is analysed for the homogeneous non-autonomous problem (4.13). It is proven that a substantial order reduction is encountered for parabolic problems, in general. For instance, for a one-dimensional initial-boundary value problem subject to a homogeneous Dirichlet boundary condition, the order of convergence with respect to the discrete L^p-norm is $2+\kappa$ where $0 \le \kappa < (2p)^{-1}$. Therefore, it seems more promising, also in view of a possible extension to quasilinear problems, to employ a suitable linearisation and to base the scheme on an explicit exponential Runge–Kutta or multistep method.

In the last years, exponential and Magnus integrators attracted a lot of interest. However, in particular in connection with parabolic problems, their practical value and competitiveness with established schemes substantially depends on an efficient implementation of the matrix exponential function. Furthermore, it is indispensable to provide a variable stepsize implementation based on an error control and to develop suitable linearisation strategies. To the latter aim, when considering semilinear problems where the linear operator A is time-independent, the results obtained in this paper seem useful.

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