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AN EXPONENTIAL INTEGRATOR FOR NON-AUTONOMOUS PARABOLIC PROBLEMS*

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Abstract. For the time integration of non-autonomous parabolic problems, a new type of exponential integrators is presented and analyzed. The construction of this integrator is closely related to general construction principles of the continuous evolution system. The proximity to the continuous problem allows one to obtain a third-order method that does not suffer from order reduction. The stated order behavior is rigorously proved in an abstract framework of analytic semigroups. The numerical behavior of the integrator is illustrated with an example that models a diffusion process on an evolving domain. Comparisons with an implicit Runge-Kutta method of order three and a standard fourth-order Magnus integrator are given.

Key words. exponential integrators, parabolic problems, time-dependent operators, evolving domains

AMS subject classifications. 65M12, 65L06

1. Introduction.

For the numerical integration of linear evolution equations of the form

$$u'(t) + A(t)u(t) = 0, \qquad u(0) = u_0, \tag{1.1}$$

Magnus integrators [1, 3, 19] are often considered to be the method of choice. This is particularly true for the linear Schrödinger equation with a smooth, time-dependent potential. Under the assumption that certain derivatives of $A(t)$ are bounded, higher-order convergence results are available; see [15]. However, it is also well-known that, in the parabolic case, Magnus integrators often suffer from order reduction, i.e., the order of convergence is reduced; see [9, 27].

In this paper, we follow a different approach in which the construction of the integrator as well as its convergence analysis are closely related to the construction of the continuous evolution system in [26]. The theory of [26] is also outlined in the monographs [8, Part 2] and [23, Section 5.6]. This proximity to the continuous problem allows one to obtain a third-order exponential integrator that does not suffer from order reduction. This integrator was first proposed in [13]. Its implementation using preconditioned Krylov subspace methods is discussed in [12]. In this paper we concentrate on the error analysis.

There are several other options for solving non-autonomous parabolic problems. For instance, discontinuous Galerkin methods in space and time [7], finite elements in space combined with BDF methods [2, 25], Runge-Kutta methods for the time discretization [10, 21], and linearly implicit methods [20, 28]. These methods, however, will not be considered further in this paper.

Non-autonomous parabolic equations as equation (1.1) arise for instance from a spatial discretization of a diffusion equation on an evolving domain. Finite element methods for parabolic differential equations on evolving surfaces were considered in [5]. Their time discretization with implicit Runge-Kutta methods was subsequently studied in [6].

The paper is organized as follows: in Section 2 we provide the analytical framework and present the construction of an approximate evolution system for (1.1). For the numerical realization we suggest a new exponential integrator; see (2.9). Section 3 contains our

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main results on error bounds for the new exponential integrator. Finally, we present numerical experiments for finite element discretizations of parabolic problems on time-dependent domains in Section 4. A comparison of the efficiency of the method using high-performance computing is beyond the scope of this paper and might be presented elsewhere.

2. Construction of an approximate evolution system. In this section we present the construction of an approximate evolution system. We work in the framework of [26] and consider (1.1) as an abstract evolution problem on a Banach space X. More precisely, we employ the following assumption:

ASSUMPTION 2.1. *The linear operators $A(t)$ are uniformly sectorial and have a common (time-invariant) domain $D\big(A(t)\big) = D$ for $t \in [0,T]$.*

Each operator $A(t)$ thus generates an analytic semigroup on X, which we denote by $\mathrm{e}^{-sA(t)}$. By a standard scaling argument, we can assume that $A(t)$ is invertible with a bounded inverse. This implies that for all $\alpha \geq 0$, there exists a constant $C > 0$ such that

$$\Big\| A(t)^{\alpha} \mathrm{e}^{-sA(t)} \Big\| \leq C s^{-\alpha}, \qquad s > 0, \tag{2.1}$$

holds uniformly in $t \in [0,T]$.

In addition, we require the Lipschitz conditions

$$\big\| \big(A(s) - A(t)\big) A(0)^{-1} \big\| \leq C\, |t-s|\,, \tag{2.2a}$$

and[1]

$$\big\| A^{-1}(0) \big(A(t) - A(s)\big) \big\| \leq C\, |t-s|\,. \tag{2.2b}$$

Let $\tau > 0$ be a fixed step size and $t_n = n\tau$, $n \in \{0,1,\ldots\}$. By [26, eq. (1.14)], the solution of (1.1) at time $t_n + \tau$ can be written as

$$\begin{aligned} u(t_n+\tau) &= G(t_n+\tau, t_n) u(t_n), \\ G(t_n+\tau, t_n) &= \mathrm{e}^{-\tau A_n} + \int_0^{\tau} \mathrm{e}^{-(\tau-s)A(t_n+s)} R(t_n+s, t_n)\,\mathrm{d}s, \end{aligned} \tag{2.3}$$

where $A_n = A(t_n)$. The operator R is defined by the integral equation

$$R(t+s,t) = R_1(t+s,t) + \int_0^s R_1(t+s, t+\sigma) R(t+\sigma, t)\,\mathrm{d}\sigma, \tag{2.4}$$

or, by [26, eq. (1.31)], as

$$R(t+s,t) = R_1(t+s,t) + \int_0^s R(t+s, t+\sigma) R_1(t+\sigma, t)\,\mathrm{d}\sigma, \tag{2.5}$$

where

$$R_1(t,s) = \big(A(s) - A(t)\big) \mathrm{e}^{-(t-s)A(s)}. \tag{2.6}$$

It was shown in [23, eq. (5.6.23)] that

$$R(t,s) = \sum_{m=1}^{\infty} R_m(t,s), \qquad \| R_m(t,s) \| \leq C\, |t-s|^{m-1}\,. \tag{2.7}$$

---
[1] Throughout the paper, we do not distinguish in notation between an operator and its closure.

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To construct a numerical method from the evolution operator (2.3), two approximations are required. First, we have to truncate the series (2.7). Here, the simplest choice is to truncate after the first term. In fact we will later see that this is sufficient to obtain order three, and thus we do not consider using more terms.

Secondly, we have to discretize the integral in (2.3). Applying a standard quadrature formula would give unfortunate error bounds involving derivatives of the integrand and thus powers of the unbounded operator A. Thus we freeze the semigroup appearing in the integral and approximate only R_1 by a polynomial. This is a particular form of an exponential quadrature rule [16, 17] using only one evaluation of the semigroup. Numerical results indicated that using A_{n+1} leads to a small error constant. However, freezing the semigroup at any time in the interval $[t_n, t_{n+1}]$ gives the same order. Altogether, this yields the following approximation to $u(t_{n+1})$:

$$
\begin{aligned}
\widetilde{u}_{n+1} &= \widetilde{G}(t_n+\tau, t_n)\widetilde{u}_n, \\
\widetilde{G}(t_n+\tau, t_n) &= \mathrm{e}^{-\tau A_n} + \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} R_1(t_n+s, t_n)\,\mathrm{d}s,
\end{aligned}
\tag{2.8}
$$

where $\widetilde{u}_0 = u_0$.

Next we replace $R_1(t_n+s, t_n)$ by an interpolation polynomial p_n of order two which is third-order accurate. A natural choice for the interpolation nodes is $c_1 = 0$ (since $R_1(t,t)=0$) and $c_3 = 1$ (because one can then reuse A_{n+1} in the next time step). Choosing some value $0 < c_2 < 1$ gives the numerical scheme

$$
u_{n+1} = T_n u_n, \qquad T_n = \mathrm{e}^{-\tau A_n} + \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} p_n(s)\,\mathrm{d}s. \tag{2.9a}
$$

The integral can be expressed explicitly in terms of the φ-functions defined as

$$
\varphi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!}\,\mathrm{d}\theta, \qquad k \in \{1, 2, \ldots\}.
$$

As an example, we choose $c_2 = 1/2$. Carrying out this integration, we obtain an explicit representation of the discrete evolution operator

$$
\begin{aligned}
T_n = \mathrm{e}^{-\tau A_n} &+ 4\tau\Big(\varphi_2(-\tau A_{n+1}) - 2\varphi_3(-\tau A_{n+1})\Big)(A_n - A_{n+1/2})\mathrm{e}^{-\frac{\tau}{2}A_n} \\
&+ \tau\Big(4\varphi_3(-\tau A_{n+1}) - \varphi_2(-\tau A_{n+1})\Big)(A_n - A_{n+1})\mathrm{e}^{-\tau A_n}.
\end{aligned}
\tag{2.9b}
$$

This completes the derivation of the numerical method. Its convergence properties will be investigated in the following section.

3. Error bounds. Motivated by the derivation above, we split the convergence proof into two parts. We first prove error bounds for the approximation (2.8), and then we consider the interpolation error to bound the error for the final approximation (2.9).

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3.1. Error bound for $\widetilde{u}_n$. Let

$$\widetilde{e}_n = u(t_n) - \widetilde{u}_n$$

denote the error of the approximation (2.8). Subtracting (2.8) from (2.3) and inserting (2.4) gives the error recursion

$$\begin{aligned}\widetilde{e}_{n+1} = \mathrm{e}^{-\tau A_n}\widetilde{e}_n &+ \int_0^\tau \mathrm{e}^{-(\tau-s)A(t_n+s)} R_1(t_n+s,t_n)u(t_n)\,\mathrm{d}s \\ &- \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} R_1(t_n+s,t_n)\widetilde{u}_n\,\mathrm{d}s \\ &+ \int_0^\tau \mathrm{e}^{-(\tau-s)A(t_n+s)} \int_0^s R_1(t_n+s,t_n+\sigma)R(t_n+\sigma,t_n)u(t_n)\,\mathrm{d}\sigma\,\mathrm{d}s.\end{aligned}$$

With the abbreviations

$$\delta_{n+1} = \delta_{n+1}^{[1]} + \delta_{n+1}^{[2]}, \tag{3.1a}$$

$$\delta_{n+1}^{[1]} = \int_0^\tau \big(\mathrm{e}^{-(\tau-s)A(t_n+s)} - \mathrm{e}^{-(\tau-s)A_{n+1}}\big)R_1(t_n+s,t_n)\,\mathrm{d}s, \tag{3.1b}$$

$$\delta_{n+1}^{[2]} = \int_0^\tau \mathrm{e}^{-(\tau-s)A(t_n+s)} \int_0^s R_1(t_n+s,t_n+\sigma)R(t_n+\sigma,t_n)\,\mathrm{d}\sigma\,\mathrm{d}s, \tag{3.1c}$$

the error recursion can be written as

$$\widetilde{e}_{n+1} = \mathrm{e}^{-\tau A_n}\widetilde{e}_n + \delta_{n+1}u(t_n) + \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} R_1(t_n+s,t_n)\,\mathrm{d}s\,\widetilde{e}_n.$$

Since $\widetilde{e}_0 = 0$, we get

$$\widetilde{e}_n = \sum_{j=0}^{n-1} \mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_{j+1}} \left(\delta_{j+1}u(t_j) + \int_0^\tau \mathrm{e}^{-(\tau-s)A_{j+1}} R_1(t_j+s,t_j)\,\mathrm{d}s\,\widetilde{e}_j\right), \tag{3.2}$$

where we used the notation $\mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_{j+1}} = I$ for $j = n-1$. A naive bound for (3.1) would give a second-order estimate only. To improve this estimate, we have to employ the smoothness of the solution $u(t)$ and the parabolic smoothing property.

We start with the following lemma.

LEMMA 3.1. *δ_{n+1} defined in (3.1) satisfies the estimates*

$$\big\|\delta_{n+1}A_n^{-1}\big\| \le C\tau^3, \qquad \big\|A_{n+1}^{-1}\delta_{n+1}A_n^{-1}\big\| \le C\tau^4. \tag{3.3}$$

Proof. Let $\theta \ge 0$. The identity

$$\mathrm{e}^{-\theta A(t)} - \mathrm{e}^{-\theta A(s)} = \int_0^\theta \mathrm{e}^{-(\theta-\sigma)A(t)}\big(A(s)-A(t)\big)\mathrm{e}^{-\sigma A(s)}\,\mathrm{d}\sigma$$

together with (2.1) and (2.2) allows us to prove the bounds

$$\begin{aligned}\Big\|\mathrm{e}^{-\theta A(t)} - \mathrm{e}^{-\theta A(s)}\Big\| &\le C\,|t-s|\,, \\ \Big\|A(t)^{-1}\big(\mathrm{e}^{-\theta A(t)} - \mathrm{e}^{-\theta A(s)}\big)\Big\| &\le C\theta\,|t-s|\,.\end{aligned}$$

The proof of the first bound is not as obvious as that of the second one and can be found in [26, eq. (1.21)]. Moreover, using the definition (2.6) of R_1 gives

$$\big\|R_1(t,s)A(s)^{-1}\big\| \le C\,|t-s|\,, \qquad \big\|A(t)^{-1}R_1(t,s)\big\| \le C\,|t-s|\,. \tag{3.4a}$$

As a consequence, (2.5), (2.7) provide us with the estimates

$$\big\|R(t,s)A(s)^{-1}\big\| \le C\,|t-s|\,, \qquad \big\|A(t)^{-1}R(t,s)\big\| \le C\,|t-s|\,. \tag{3.4b}$$

These estimates prove the first inequality in (3.3).

The proof of the second one is obtained from

$$\Big\|A_{n+1}^{-1}\delta_{n+1}^{[1]}A_n^{-1}\Big\| \le C\int_0^\tau (\tau-s)^2 s\,\mathrm{d}s \le C\tau^4$$

and, using the estimates (3.4a) and (3.4b), by

$$\Big\|A(t_n+s)^{-1}\delta_{n+1}^{[2]}A_n^{-1}\Big\| \le C\int_0^\tau\int_0^s (s-\sigma)\sigma\ \mathrm{d}\sigma\ \mathrm{d}s \le C\tau^4.$$

The claim now follows from $\big\|A_{n+1}^{-1}A(t_n+s)\big\| \le C$ and the triangle inequality. ∎

By (2.7), we also have

$$\left\|\int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}}R_1(t_n+s,t_n)\,\mathrm{d}s\right\| \le C\tau. \tag{3.5}$$

In addition to these bounds we will need certain stability results. The key idea to prove stability is to write

$$\Delta_{n,j} = G(t_n,t_j) - \mathrm{e}^{-\tau A_{n-1}}\cdots\mathrm{e}^{-\tau A_j}, \qquad j<n, \qquad \Delta_{n,n}=0 \tag{3.6}$$

as a telescopic sum; see [22]. From [26, eq. (1.77)], we have the local error bound

$$\Big\|A^{-\alpha}(t)\big(G(t,s)-\mathrm{e}^{-(t-s)A(s)}\big)A^{\beta}(s)\Big\| \le C\,|t-s|^{1+\alpha-\beta}, \qquad 0\le\alpha,\beta\le 1. \tag{3.7}$$

Moreover [26, Theorem 3] shows that

$$\big\|A^{-\alpha}(t)G(t,s)A^{\beta}(s)\big\| \le C\,|t-s|^{\alpha-\beta}, \qquad 0\le\alpha\le\beta<2, \tag{3.8a}$$

$$\big\|A^{\alpha}(t)G(t,s)A^{\beta}(s)\big\| \le C\,|t-s|^{-\alpha-\beta}, \qquad 0\le\alpha,\beta<2. \tag{3.8b}$$

LEMMA 3.2. *For $0\le j\tau<n\tau\le T$ we have*

$$\big\|\mathrm{e}^{-\tau A_{n-1}}\cdots\mathrm{e}^{-\tau A_j}\big\| \le C,$$

where C depends on T but is independent of τ, n, and j.

Proof. We use the telescopic identity to write (3.6) as

$$\begin{aligned}\Delta_{n,j} &= \sum_{i=j+1}^{n} \mathrm{e}^{-\tau A_{n-1}}\cdots\mathrm{e}^{-\tau A_i}\big(G(t_i,t_{i-1})-\mathrm{e}^{-\tau A_{i-1}}\big)G(t_{i-1},t_j)\\ &= \sum_{i=j+1}^{n} \big(G(t_n,t_i)-\Delta_{n,i}\big)\big(G(t_i,t_{i-1})-\mathrm{e}^{-\tau A_{i-1}}\big)G(t_{i-1},t_j).\end{aligned} \tag{3.9}$$

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The uniform boundedness of the exact propagator $G(t,s)$ (see (3.8a) for $\alpha = \beta = 0$) yields

$$\|\Delta_{n,j}\| \le C\tau \sum_{i=j+1}^{n} \big(C + \|\Delta_{n,i}\|\big) \le C + C\tau \sum_{i=j+1}^{n} \|\Delta_{n,i}\| \,.$$

Applying a variant of the discrete Gronwall lemma shows that $\|\Delta_{n,j}\| \le C$. This completes the proof. ∎

LEMMA 3.3. *For $0 \le j\tau < n\tau \le T$ we have*

$$(t_n - t_j)\, \big\|\mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_j} A_j\big\| \le C(1 + |\log \tau|), \tag{3.10}$$

where C depends on T but is independent of τ, n, and j.

Proof. We insert factors of the form $A_k A_k^{-1}$ into the telescopic identity (3.9). Then (3.7), (3.8a), and the triangle inequality immediately give

$$\|\Delta_{n,j} A_j\| \le C\tau \sum_{i=j+1}^{n-1} \big((t_n - t_i)^{-1} + \|\Delta_{n,i} A_i\|\big) + C.$$

A discrete Gronwall lemma then shows that $\|\Delta_{n,j} A_j\| \le C(1 + |\log \tau|)$. The desired bound thus follows from (3.6) by the triangle inequality and (3.8b). ∎

Now having all these results at hand, we can bound the error for (2.8).

THEOREM 3.4. *Let Assumption 2.1 and (2.2) be satisfied and assume that the solution u of (1.1) satisfies $u \in C^1([0,T], X)$. Then the error bound*

$$\|u(t_n) - \widetilde{u}_n\| \le C\tau^3 (1 + |\log \tau|)^2 \max_{t\in[0,T]} \|u'(t)\| \,, \tag{3.11}$$

holds for $0 \le t_n = n\tau \le T$, where C is a constant which is independent of n and τ.

Proof. We start from the error recursion (3.2)

$$\begin{aligned}
\|\widetilde{e}_n\| \le \sum_{j=0}^{n-2} &\big\|\mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_{j+1}} A_{j+1}\big\| \, \big\|A_{j+1}^{-1} \delta_{j+1} A_j^{-1}\big\| \, \|A_j u(t_j)\| \\
&+ \sum_{j=0}^{n-1} \big\|\mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_{j+1}}\big\| \, \left\| \int_0^\tau \mathrm{e}^{-(\tau - s) A_{j+1}} R_1(t_j + s, t_j)\, \mathrm{d}s \right\| \|\widetilde{e}_j\| \\
&+ \big\|\delta_n A_{n-1}^{-1}\big\| \, \|A_{n-1} u(t_{n-1})\| \,.
\end{aligned}$$

Using the stability results from Lemmas 3.2 and 3.3 and the bounds (3.3) and (3.5), we obtain

$$\begin{aligned}
\|\widetilde{e}_n\| &\le C \sum_{j=0}^{n-2} \frac{1 + |\log \tau|}{t_n - t_{j+1}} \tau^4 \, \|A_j u(t_j)\| + C\tau \sum_{j=0}^{n-1} \|\widetilde{e}_j\| + C\tau^3 \, \|A_{n-1} u(t_{n-1})\| \\
&\le C\tau^3 (1 + |\log \tau|)^2 \max_{t\in[0,T]} \|A(t) u(t)\| + C\tau \sum_{j=0}^{n-1} \|\widetilde{e}_j\| \,.
\end{aligned}$$

Another application of the discrete Gronwall lemma establishes the desired error-bound. ∎

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3.2. Error bound for u_n. It remains to study the quadrature error which arises from replacing

$$g_n(s) = R_1(t_n + s, t_n)$$

in (2.8) by its interpolation polynomial p_n leading to the approximation (2.9). The total error can be decomposed into

$$e_n = u(t_n) - u_n = \widehat{e}_n + \widetilde{e}_n, \qquad \widehat{e}_n = \widetilde{u}_n - u_n,$$

where the quadrature error $\widehat{e}_n$ satisfies the recursion

$$\begin{aligned}\widehat{e}_{n+1} = \mathrm{e}^{-\tau A_n}\widehat{e}_n &+ \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}}\big(g_n(s) - p_n(s)\big)\widetilde{u}_n \,\mathrm{d}s \\ &+ \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} p_n(s)\widehat{e}_n \,\mathrm{d}s.\end{aligned}$$

Bounding the quadrature error requires the map $t \mapsto A(t)A(0)^{-1}$ to be four times differentiable with bounded derivatives, i.e.,

$$\left\| A^{(k)}(t)A(s)^{-1} \right\| \le C, \qquad 0 \le s,t \le T, \qquad k = 0,1,\ldots,4. \tag{3.12}$$

Note that this condition implies (2.2a).

Using the abbreviations

$$\chi_{n+1} = \widetilde{G}(t_{n+1}, t_n) - T_n = \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}}\big(g_n(s) - p_n(s)\big)\,\mathrm{d}s \tag{3.13a}$$

and

$$\beta_{n+1} = \int_0^\tau \mathrm{e}^{-(\tau-s)A_{n+1}} p_n(s)\,\mathrm{d}s, \tag{3.13b}$$

we rewrite the error recursion as

$$\begin{aligned}\widehat{e}_{n+1} &= \mathrm{e}^{-\tau A_n}\widehat{e}_n + \beta_{n+1}\widehat{e}_n + \chi_{n+1}\widetilde{u}_n \\ &= \mathrm{e}^{-\tau A_n}\widehat{e}_n + \beta_{n+1}\widehat{e}_n - \chi_{n+1}\widetilde{e}_n + \chi_{n+1}u(t_n).\end{aligned}$$

As $\widehat{e}_0 = 0$, we have

$$\widehat{e}_n = \sum_{j=0}^{n-1} \mathrm{e}^{-\tau A_{n-1}} \cdots \mathrm{e}^{-\tau A_{j+1}}\big(\beta_{j+1}\widehat{e}_j - \chi_{j+1}\widetilde{e}_j + \chi_{j+1}u(t_j)\big). \tag{3.14}$$

We start with a counterpart of Lemma 3.1.

LEMMA 3.5. *χ_{n+1} defined in (3.13a) satisfies the estimates*

$$\left\|\chi_{n+1}A_n^{-2}\right\| \le C\tau^3, \qquad \left\|A_{n+1}^{-1}\chi_{n+1}A_n^{-2}\right\| \le C\tau^4. \tag{3.15}$$

Proof. Note that by definition of p_n, we have $p_n(0) = g_n(0) = 0$. We define

$$g_n(s) = s\widetilde{g}_n(s), \qquad p_n(s) = s\widetilde{p}_n(s),$$

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such that $\widetilde{p}_n$ is the interpolation polynomial of $\widetilde{g}_n$ interpolating in the nodes $c_2\tau$ and $c_3\tau$. We will show below that the function f_n defined by

$$s \mapsto f_n(s) = A_{n+1}^{-1}\widetilde{g}_n(s)A_n^{-2}$$

satisfies $f_n \in C^2\big([0,\tau];\mathcal{L}(X)\big)$. Thus the interpolation error can be estimated by

$$\big\|A_{n+1}^{-1}\big(\widetilde{g}_n(s) - \widetilde{p}_n(s)\big)A_n^{-2}\big\| \le |s-c_2\tau|\,|s-c_3\tau|\,\frac{1}{2}\max_{0\le\rho\le\tau}\big\|A_{n+1}^{-1}\widetilde{g}_n''(\rho)A_n^{-2}\big\|$$

(see [4, Example 3.1]), so that we obtain the bound

$$\begin{aligned}
\big\|A_{n+1}^{-1}\chi_{n+1}A_n^{-2}\big\| &\le \int_0^\tau \Big\|A_{n+1}^{-1}\mathrm{e}^{-(\tau-s)A_{n+1}}\big(g_n(s)-p_n(s)\big)A_n^{-2}\Big\|\,\mathrm{d}s\\
&\le \tau\max_{0\le\sigma\le\tau}\Big\|\mathrm{e}^{-(\tau-\sigma)A_{n+1}}\sigma A_{n+1}^{-1}\big(\widetilde{g}_n(\sigma)-\widetilde{p}_n(\sigma)\big)A_n^{-2}\Big\|\\
&\le C\tau\max_{0\le\sigma\le\tau}\big|\sigma(\sigma-c_2\tau)(\sigma-c_3\tau)\big|\max_{0\le\rho\le\tau}\big\|A_{n+1}^{-1}\widetilde{g}_n''(\rho)A_n^{-2}\big\|\\
&\le C\tau^4\max_{0\le\rho\le\tau}\|f_n''(\rho)\|\,.
\end{aligned}$$

It remains to show that

$$\|f_n''(\rho)\| = \big\|A_{n+1}^{-1}\widetilde{g}_n''(\rho)A_n^{-2}\big\| \le C. \tag{3.16}$$

Let $A_n^{(k)} = A^{(k)}(t_n)$. In a first step we derive a different representation of $\widetilde{g}_n$:

$$\begin{aligned}
\widetilde{g}_n(s) &= \frac{1}{s}\big(A_n - A(t_n+s)\big)\,\mathrm{e}^{-sA_n}\\
&= -\frac{1}{s}\int_0^s A'(t_n+\rho)\,\mathrm{d}\rho\,\mathrm{e}^{-sA_n}\\
&= -\frac{1}{s}\int_0^s\Big(A_n' + \rho A_n'' + \frac{\rho^2}{2}A_n^{(3)} + \int_0^\rho \frac{(\rho-\sigma)^2}{2}A^{(4)}(t_n+\sigma)\,\mathrm{d}\sigma\Big)\,\mathrm{d}\rho\,\mathrm{e}^{-sA_n}\\
&= -\left(A_n' + \frac{s}{2}A_n'' + \frac{s^2}{6}A_n^{(3)} + \varrho_n(s)\right)\mathrm{e}^{-sA_n},
\end{aligned}$$

where

$$\varrho_n(s) = \frac{1}{s}\int_0^s\int_0^\rho \frac{(\rho-\sigma)^2}{2}A^{(4)}(t_n+\sigma)\,\mathrm{d}\sigma\,\mathrm{d}\rho.$$

The following derivatives are needed in the forthcoming estimates:

$$\begin{aligned}
-\widetilde{g}_n'(s) &= \widetilde{g}_n(s)A_n + \Big(\frac{1}{2}A_n'' + \frac{s}{3}A_n^{(3)} + \varrho_n'(s)\Big)\mathrm{e}^{-sA_n},\\
-\widetilde{g}_n''(s) &= \widetilde{g}_n(s)A_n^2 + 2\widetilde{g}_n'(s)A_n + \Big(\frac{1}{3}A_n^{(3)} + \varrho_n''(s)\Big)\mathrm{e}^{-sA_n},\\
\varrho_n'(s) &= \frac{1}{s}\int_0^s \frac{(s-\sigma)^2}{2}A^{(4)}(t_n+\sigma)\,\mathrm{d}\sigma - \frac{1}{s}\varrho_n(s),\\
\varrho_n''(s) &= -\frac{2}{s}\varrho_n'(s) + \frac{1}{s}\int_0^s (s-\sigma)A^{(4)}(t_n+\sigma)\,\mathrm{d}\sigma.
\end{aligned}$$

Now we begin with the proof of (3.16). The remainder terms can be handled as

$$\begin{aligned}
\left\|\varrho_n(s)A_n^{-1}\right\| &\le \frac{1}{s}\int_0^s\int_0^\rho \frac{(\rho-\sigma)^2}{2}\left\|A^{(4)}(t_n+\sigma)A_n^{-1}\right\| \,\mathrm{d}\sigma\,\mathrm{d}\rho \le Cs^3,\\
\left\|\varrho_n'(s)A_n^{-1}\right\| &\le \frac{1}{s}\int_0^s \frac{(s-\sigma)^2}{2}\left\|A^{(4)}(t_n+\sigma)A_n^{-1}\right\| \,\mathrm{d}\sigma + \frac{1}{s}\left\|\varrho_n(s)A_n^{-1}\right\| \le Cs^2,\\
\left\|\varrho_n''(s)A_n^{-1}\right\| &\le \frac{2}{s}\left\|\varrho_n'(s)A_n^{-1}\right\| + \frac{1}{s}\int_0^s (s-\sigma)\left\|A^{(4)}(t_n+\sigma)A_n^{-1}\right\| \,\mathrm{d}\sigma \le Cs.
\end{aligned}$$

We continue by estimating the terms in $f_n''(s) = A_{n+1}^{-1}\widetilde{g}_n''(s)A_n^{-2}$ one after another. For the first two terms we have by (3.12)

$$\begin{aligned}
\left\|A_{n+1}^{-1}\widetilde{g}_n(s)\right\| &\le \frac{C}{s}\left\|A_{n+1}^{-1}\big(A_n - A(t_n+s)\big)\right\| \le C,\\
\left\|A_{n+1}^{-1}\widetilde{g}_n'(s)A_n^{-1}\right\| &\le \left\|A_{n+1}^{-1}\widetilde{g}_n(s)\right\| + C\left\|\Big(\frac{1}{2}A_n'' + \frac{s}{3}A_n^{(3)} + \varrho_n'(s)\Big)A_n^{-1}\right\| \le C,
\end{aligned}$$

while the last term is bounded by

$$\left\|A_{n+1}^{-1}\Big(\frac{1}{3}A_n^{(3)} + \varrho_n''(s)\Big)A_n^{-2}\mathrm{e}^{-sA_n}\right\| \le C.$$

This proves the second estimate in (3.15).

For the first one it suffices to consider the interpolation error for only one interpolation node and thus to bound the first derivative of $\widetilde{g}_n(s)A_n^{-2}$. Since all these bounds are obtained completely analogously, this completes the proof. □

THEOREM 3.6. *Let Assumption 2.1, (2.2b), and (3.12) be satisfied and let u be the solution of (1.1). If $u \in C^2([0,T],X)$, then the error bound*

$$\|u(t_n) - u_n\| \le C\tau^3\big(1+|\log\tau|\big)^2\left(\max_{t\in[0,T]}\|u'(t)\| + \max_{t\in[0,T]}\|u''(t)\|\right)$$

holds for $0 \le t_n = n\tau \le T$, where C is a constant that is independent of n and τ.

Proof. Inserting the obvious bounds

$$\|\beta_{n+1}\| \le C\tau, \qquad \|\chi_{n+1}\| \le C\tau,$$

the estimates (3.15) and the stability bound (3.10) into the error recursion (3.14) gives

$$\begin{aligned}
\|\widehat{e}_n\| \le C\tau\sum_{j=0}^{n-1}\|\widehat{e}_j\| + C\max_{0\le j\le n-1}\|\widetilde{e}_n\|\\
+ C\sum_{j=0}^{n-2}\frac{1+|\log\tau|}{t_n-t_j}\tau^4\left\|A_j^2u(t_j)\right\| + C\tau^3\left\|A_{n-1}^2u(t_{n-1})\right\|.
\end{aligned}$$

Using (3.11) and applying a Gronwall argument proves the desired result. □

4. Parabolic problems on time-dependent domains. To illustrate the theoretical results of this paper, we apply our method to a finite element discretization of a diffusion equation on an evolving domain (DEED) in $\mathbb{R}^2$. Our formulation, analysis, and spatial discretization of DEED is motivated by [5], where semi-discretizations of parabolic problems on evolving surfaces are considered.

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4.1. The diffusion equation on an evolving domain. Consider a scalar quantity u defined on the time-space domain

$$\mathcal{N}_T = \bigcup_{t\in[0,T]} \{t\} \times \Omega_t,$$

where the evolution of $\Omega_t \subset \mathbb{R}^2$ is given by a family of diffeomorphisms X_t between a bounded domain Ω_0 and its images Ω_t, $t \in [0,T]$. The material time derivative of a function $v : \mathcal{N}_T \to \mathbb{R}$ with respect to X_t is given by

$$D_t v(t,x) = \frac{\mathrm{d}}{\mathrm{d}t}\big(v(t,X_t(y))\big)\Big|_{y=X_t^{-1}(x)};$$

see [5] for details. With this notation we define the function space

$$V = \big\{v : \mathcal{N}_T \to \mathbb{R}\ ;\ v(t,\cdot) \in H_0^1(\Omega_t),\ D_t v(t,\cdot) \in L^2(\Omega_t) \text{ for all } t \in [0,T]\big\}.$$

The weak formulation of a diffusion equation on the evolving domain Ω_t can be stated as follows: find $u \in V$ such that for all $t \in (0,T]$ and all $v \in V$ the equality

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} uv\,\mathrm{d}x + \alpha\int_{\Omega_t} \nabla u\cdot\nabla v\,\mathrm{d}x = \int_{\Omega_t} uD_t v\,\mathrm{d}x, \tag{4.1}$$

holds subject to the initial condition $u(0,\cdot) = u_0$ and to homogeneous Dirichlet boundary conditions $u(t,x) = 0$ for all $x \in \partial\Omega_t$. The number $\alpha > 0$ denotes the diffusion constant.

For the spatial discretization of (4.1), we use linear finite elements. Let $\mathcal{T}_0$ be a triangulation of Ω_0 with nodes $a_1,\ldots,a_K$ and nodal basis functions $\phi_1,\ldots,\phi_K$. By h we denote the maximum diameter of its triangles. Starting from $\mathcal{T}_0$ we define an approximate evolving domain $\Omega_t^h = X_{t,h}(\Omega_0)$, where

$$X_{t,h}(y) = \sum_{i=1}^{K} \phi_i(y)X_t(a_i) \approx X_t(y), \quad y \in \Omega_0.$$

By this construction, Ω_t^h gets equipped with a triangulation. The corresponding basis functions $\Phi_i \in V$ are then given by $\Phi_i(t,x) = \phi_i(X_{t,h}^{-1}(x))$. They satisfy in particular $D_t\Phi_i = 0$, where the material derivative is taken with respect to $X_{t,h}$. The function spaces $V_h = \operatorname{span}\{\Phi_1,\ldots,\Phi_K\}$ and

$$U_h = \left\{u : u(t,\cdot) = \sum_{i=1}^{K} U_i(t)\Phi_i(t,\cdot),\ U_i \in C^1\big([0,T],\mathbb{R}\big)\right\}$$

fulfill $V_h \subset U_h$. Note that the dimension of V_h is independent of t by construction. The semi-discrete solution $u_h \in U_h$ then solves the variational problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t^h} u_h\,\psi_h\,\mathrm{d}x \,+\, \alpha\int_{\Omega_t^h} \nabla u_h\cdot\nabla\psi_h\,\mathrm{d}x \,=\, \int_{\Omega_t^h} u_h\,D_t\psi_h\,\mathrm{d}x \,=\, 0 \tag{4.2}$$

for all $\psi_h \in V_h$ and $t \in [0,T]$. In [11] it was shown that $u_h(t)$ is at least a first-order approximation to the solution of (4.1) in the L^2-norm. The homogeneous Dirichlet boundary condition can be dealt with by dimension reduction of the occurring matrices. Let $\mathbf{u}(t)$ be the coefficient vector containing the coefficients $U_i(t)$ with respect to the basis functions $\Phi_i(t,\cdot)$

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that correspond to the interior nodes of Ω_t^h. From (4.2) we then obtain the stiff system of ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\mathbf{M}_h(t)\mathbf{u}(t)\Big) + \mathbf{S}_h(t)\mathbf{u}(t) = 0, \qquad \mathbf{u}(0) = \mathbf{u}_0, \tag{4.3}$$

where $\mathbf{M}_h(t)$ and $\mathbf{S}_h(t)$ denote the mass and stiffness matrices, respectively.

In order to rewrite (4.3) in the form (1.1), we apply the transformation

$$\mathbf{y}(t) = \mathbf{M}_h(t)\mathbf{u}(t) \tag{4.4}$$

and obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{y}(t) + \mathbf{S}_h(t)\big(\mathbf{M}_h(t)\big)^{-1}\mathbf{y}(t) = 0, \qquad \mathbf{y}(0) = \mathbf{M}_h(0)\mathbf{u}_0. \tag{4.5}$$

Hence, we end up with problem (1.1) where the operator $A(t)$ is represented by the matrix

$$\mathbf{A}(t) = \mathbf{S}_h(t)\big(\mathbf{M}_h(t)\big)^{-1}.$$

Since

$$\|u_h(t)\|^2_{L^2(\Omega_t^h)} = \mathbf{u}(t)^{\mathsf{T}}\mathbf{M}_h(t)\mathbf{u}(t), \tag{4.6}$$

the norm

$$\|\mathbf{y}\|^2_{t,h} = \mathbf{y}^{\mathsf{T}}\big(\mathbf{M}_h(t)\big)^{-1}\mathbf{y} = \|u_h\|^2_{L^2(\Omega_t^h)}$$

is the appropriate one for the transformed variables $\mathbf{y}$ in $\mathbb{R}^d$. Our assumptions on the family $\{X_t\}_{t\in[0,T]}$ imply that $\|\cdot\|_{t,h}$ is uniformly equivalent to $\|\cdot\|_{0,h}$ for all $t \in [0,T]$. We thus write $\|\cdot\| = \|\cdot\|_{0,h}$ for simplicity.

If the exponential integrator is implemented with a polynomial or rational Krylov subspace method, it should be written in the form

$$\begin{aligned}
\widetilde{\mathbf{y}}_{n+1/2} &= \exp\left(-\tfrac{\tau}{2}\mathbf{M}_n^{-1}\mathbf{S}_n\right)\mathbf{u}_n,\\
\widetilde{\mathbf{y}}_{n+1} &= \exp\left(-\tau\mathbf{M}_n^{-1}\mathbf{S}_n\right)\mathbf{u}_n,\\
\widetilde{\mathbf{u}}_{n+1} &= \mathbf{M}_{n+1}^{-1}\mathbf{M}_n\widetilde{\mathbf{y}}_{n+1},\\
\widetilde{\mathbf{z}}_{n+1/2} &= \mathbf{M}_{n+1}^{-1}\Big(\mathbf{S}_n\widetilde{\mathbf{y}}_{n+1/2} - \mathbf{S}_{n+1/2}\mathbf{M}_{n+1/2}^{-1}\mathbf{M}_n\widetilde{\mathbf{y}}_{n+1/2}\Big),\\
\widetilde{\mathbf{z}}_{n+1} &= \mathbf{M}_{n+1}^{-1}\Big(\mathbf{S}_n\widetilde{\mathbf{y}}_{n+1} - \mathbf{S}_{n+1}\widetilde{\mathbf{u}}_{n+1}\Big),\\
\mathbf{u}_{n+1} &= \widetilde{\mathbf{u}}_{n+1} + \Phi_1\left(-\tau\mathbf{M}_{n+1}^{-1}\mathbf{S}_{n+1}\right)\left(4\tau\widetilde{\mathbf{z}}_{n+1/2}\right) + \Phi_2\left(-\tau\mathbf{M}_{n+1}^{-1}\mathbf{S}_{n+1}\right)\left(\tau\widetilde{\mathbf{z}}_{n+1}\right),
\end{aligned}$$

where $\mathbf{M}_n = \mathbf{M}_h(t_n)$, $\mathbf{S}_n = \mathbf{S}_h(t_n)$, $\Phi_1(z) = \varphi_2(z) - 2\varphi_3(z)$, and $\Phi_2(z) = 4\varphi_3(z) - \varphi_2(z)$. This reformulation requires only one expensive Krylov approximation, namely the approximations of $\widetilde{\mathbf{y}}_{n+1}$ and $\widetilde{\mathbf{y}}_{n+1/2}$, which can be computed in the same Krylov subspace. All other matrix approximations or solutions of linear systems are cheap because they use a small right-hand side vector of size $\mathcal{O}(\tau)$ or a good starting vector is available. In both cases, the conjugate gradient method converges in only few steps even without preconditioning if τ is not too large. For more details, we refer to [12].

It would be rather tedious and technical to rigorously verify the assumptions of Theorem 3.6 for the discretized problem. Therefore, we restrict ourselves to an illustration of the results by numerical experiments for a donut-shaped domain. For a different example we refer to [13].

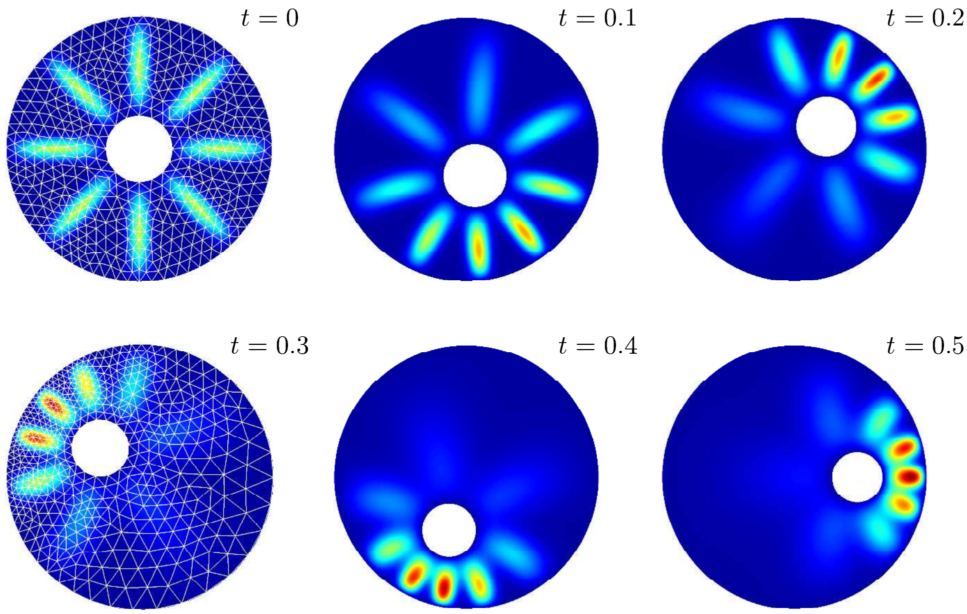

FIG. 4.1. *Snapshots of the solution on a triangulation with* $31\,842$ *nodes. For* $t = 0$ *and* $t = 0.3$ *the plots are layered with a much coarser mesh to illustrate the evolution of the domain.*

4.2. Example. We consider the circular domain with a circular hole given by $\Omega_0 = \operatorname{int}\big(B_1(0) \setminus B_{1/4}(0)\big)$, where $B_r(x)$ denotes the ball with center x and radius r. To simplify the presentation, we identify $\mathbb{R}^2$ and $\mathbb{C}$ and do not distinguish between a vector $x \in \mathbb{R}^2$ and the complex number $z = x_1 + \mathrm{i}x_2 \in \mathbb{C}$. The diffeomorphism X_t is constructed from the conformal mapping $\Lambda(z, z_0) = (z - z_0)/(1 - z\,\overline{z}_0)$. For $|z_0| < 1$, $\Lambda(\cdot, z_0)$ maps the complex unit ball onto itself. In order to construct an evolving domain we move the center z_0 of the hole along the curve $t \mapsto z_0(t) = \sqrt{t/2}\,\mathrm{e}^{6\mathrm{i}\pi t}$ describing a spiral. This gives the transformation

$$X_t(x) = (\operatorname{Re} w, \operatorname{Im} w), \qquad w = \Lambda(x_1 + \mathrm{i}x_2, z_0(t)).$$

The initial value u_0 is given by

$$u_0(x) = \begin{cases} \frac{16}{9}\big(1 - \|x\|\big)\big(4\,\|x\| - 1\big)\big(1 - 8\operatorname{dist}(x, \mathcal{S})\big), & \operatorname{dist}(x, \mathcal{S}) < \frac{1}{8}, \\ 0, & \text{otherwise,} \end{cases}$$

for $\mathcal{S} = \big\{s\mathrm{e}^{\mathrm{i}k\pi/4}\,;\, s \in [0, 1], k = 0, \ldots, 7\big\}$. Some snapshots of the solution of are shown in Figure 4.1. A movie can be found here[2] and, with a typical triangulation, here[3].

4.3. Numerical comparison. We now compare the convergence behavior of our new exponential integrator ExpInt with that of an implicit Runge-Kutta method of classical order three (the 2-stage Radau IIA method; see [10, Sec. IV.5]), and with a Magnus integrator [1] of classical order four. We only show the results for the Magnus integrator based on the

[2]Url: `http://etna.math.kent.edu/vol.41.2014/pp497-511.dir/DiffusDonut.avi`
[3]Url: `http://etna.math.kent.edu/vol.41.2014/pp497-511.dir/DiffusDonut_mesh.avi`

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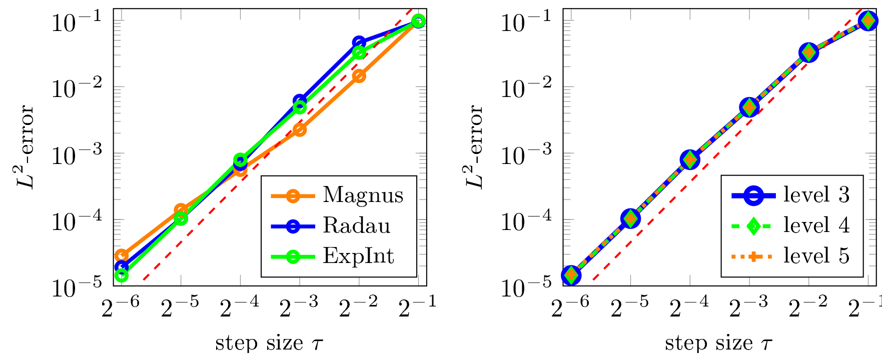

FIG. 4.2. *Left: Error versus step size for the mesh corresponding to level* 3 *(2052 DOFs) at* $t = 0.5$ *for* $\alpha = 0.01$. *Right: Errors of the exponential integrator for meshes of refinement level* 3 *(2052 DOFs), level* 4 *(8040 DOFs), and level* 5 *(31824 DOFs) at* $t = 0.5$ *for* $\alpha = 0.01$. *In both graphs, the red dashed line indicates convergence of order three.*

Simpson rule [1, eq. (256)]. Computationally, this method is more efficient than the Magnus method based on Gauss–Legendre quadrature [1, eq. (254)], and both give more or less the same results. For a comparison of the efficiency of these integrators, careful implementations of the involved linear algebra issues are indispensable for all methods. Hence we omit such comparisons here.

For Radau IIA methods, the error analysis of [20, Theorem 3.2] applies, which shows that the method with two stages converges with order three. Note that implicit Runge-Kutta methods can be applied to (4.3) directly while the Magnus integrator and the exponential integrator require the explicit formulation (4.5). From the analysis presented in [27], it is known that Magnus methods can suffer from strong order reduction when applied to parabolic problems.

In order to be able to compute problems on very fine grids, we used the GMRES method [24] to solve the linear systems arising in the Runge-Kutta scheme. For the Magnus method and the exponential integrator, we used a polynomial Krylov subspace method based on the symmetric Lanczos process for the approximations of the products of matrix functions with vectors, see [14] for an analysis of the convergence properties. It is important to use the correct inner product for the orthogonalization process. Note that by means of the transformation (4.4) we can write

$$\varphi\big(-\tau \mathbf{S}_h \mathbf{M}_h^{-1}\big)\mathbf{y} = \mathbf{M}_h \varphi\big(-\tau \mathbf{M}_h^{-1}\mathbf{S}_h\big)\mathbf{u}.$$

(We omit the argument t for the moment.) We then compute an approximation in the Krylov subspace with respect to the matrix $\mathbf{M}_h^{-1}\mathbf{S}_h$ and the vector $\mathbf{u}$. The Lanczos basis is orthonormal with respect to the norm (4.6) induced by the inner product $(\mathbf{u}\,|\,\mathbf{v}) = \mathbf{u}^{\mathsf{T}}\mathbf{M}_h\mathbf{v}$. The detailed algorithm for the approximation of the exponential function involving a mass matrix can be found in [18].

The error is determined with the help of a reference solution computed with the 3-stage Radau IIA method of classical order five using a small time step $\tau = 0.005$.

In the left graph of Figure 4.2 we plotted the error of the approximation at $t = 0.5$ versus the time step size τ on the mesh level three (2052 DOFs). As expected, the Runge-Kutta method and the exponential integrator show order three. The effect of the logarithmic term in the error bound of Theorem 3.6 is negligible. The numerically observed order of the Magnus integrator is approximately two, i.e., it suffers from a strong order reduction.

The right graph of Figure 4.2 shows errors of the exponential integrator applied to (4.5) at $t = 0.5$ for different meshes. Clearly, the error is independent of the spatial mesh width h. The same is true for the Runge-Kutta code although we have not included these results in the picture for the sake of presentation.

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