

ON THE CONVERGENCE OF SPLIT EXPONENTIAL INTEGRATORS FOR SEMILINEAR PARABOLIC PROBLEMS*

MARCO CALIARI[†], FABIO CASSINI[‡], LUKAS EINKEMMER[§],
AND ALEXANDER OSTERMANN[¶]

Abstract. Splitting the exponential-like φ functions, which typically appear in exponential integrators, is attractive in many situations since it can dramatically reduce the computational cost of the procedure. However, depending on the employed splitting, this can result in order reduction. The aim of this paper is to analyze different such split approximations. We perform the analysis for semilinear problems in the abstract framework of commuting semigroups and derive error bounds that depend, in particular, on whether the vector (to which the φ functions are applied) satisfies appropriate boundary conditions. We then present the convergence analysis for two split versions of a second-order exponential Runge–Kutta integrator in the context of analytic semigroups, and show that one suffers from order reduction while the other does not. Numerical results for semidiscretized parabolic PDEs confirm the theoretical findings.

Key words. exponential integrators, stiff equations, split approximations, order reduction, semilinear parabolic problems

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1. Introduction. The effective numerical time integration of stiff evolution differential equations is a highly challenging and widely studied topic in numerical analysis. In this context, exponential integrators have proven to be efficient methods. Indeed, the numerical solution of many physically relevant equations has been computed by this kind of schemes. We mention here, among others, magnetohydrodynamic equations, models for meteorology and elastodynamics, hyperbolic problems, and various types of advection-diffusion-reaction, Schrödinger and complex Ginzburg–Landau equations (see, e.g., [10, 13, 16, 19, 20, 22, 26]). Researchers have also put a lot of effort in the theoretical study of integrators of exponential type, and we refer to the seminal survey [18] for a comprehensive overview.

In this manuscript we are interested in semilinear parabolic problems of the type

$$(1.1) \quad \begin{cases} \partial_t u(t) = (A + B)u(t) + g(u(t)), & t \in (0, T], \\ u(0) = u_0, \end{cases}$$

where u is the unknown, A and B are differential operators that *commute* (for example, directional operators like $A = \partial_{xx}$ and $B = \partial_{yy}$ with homogeneous Dirichlet boundary conditions on a square domain) and g is the nonlinear term. Note that the operators in (1.1) are always understood with boundary conditions, and that the unknown, the

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[†]Department of Computer Science, University of Verona, Italy (marco.caliari@univr.it).

[‡]Department of Mathematics “Tullio Levi-Civita”, University of Padua, Italy (fabio.cassini@unipd.it).

[§]Department of Mathematics, University of Innsbruck, Austria (lukas.einkemmer@uibk.ac.at).

[¶]Digital Science Center, University of Innsbruck, Austria (alexander.ostermann@uibk.ac.at).

initial condition and the nonlinear term may also depend on the spatial variables (the dependence is omitted for simplicity of notation). The analytical solution of (1.1) can be written by the variation-of-constants formula as

$$(1.2) \quad u(t) = e^{t(A+B)}u_0 + \int_0^t e^{(t-s)(A+B)}g(u(s))ds,$$

which is usually the starting point for the development of exponential integrators. The commutativity of the operators A and B implies

$$(1.3) \quad e^{t(A+B)}u_0 = e^{tA}e^{tB}u_0 = e^{tB}e^{tA}u_0.$$

Note that if we consider $g(u(t)) \equiv v$ in (1.1), the solution of the (linear) problem can be written as

$$(1.4) \quad u(t) = e^{tA}e^{tB}u_0 + t\varphi_1(t(A+B))v, \quad \varphi_1(z) = \int_0^1 e^{(1-\theta)z}d\theta.$$

Clearly, even if A and B do commute, the function φ_1 lacks the semigroup property, and in general

$$(1.5) \quad t\varphi_1(t(A+B))v \neq t\varphi_1(tA)\varphi_1(tB)v = t\varphi_1(tB)\varphi_1(tA)v.$$

On the other hand, when applying exponential integrators to stiff systems of ODEs arising from the semidiscretization in space of problems of type (1.1), it could be computationally attractive to employ split formulas such as the second (or the third) expression in (1.3) and (1.5) (see, for example, [5, 6, 9]). Indeed, a classical way to recover an approximation to solution (1.4) is to apply the Strang splitting scheme to the exact flows of

$$\partial_t u_a(t) = Au_a(t), \quad \partial_t u_b(t) = Bu_b(t) + v,$$

obtaining at the first time step $t_1 = \tau$

$$(1.6) \quad u(\tau) \approx u_1 = e^{\tau A}e^{\tau B}u_0 + \tau e^{\frac{\tau}{2}A}\varphi_1(\tau B)v.$$

It is easy to verify numerically that such an approximation is subject to order reduction if the function v and/or its derivatives do not satisfy the boundary conditions. Indeed, consider $A = \partial_{xx}$ and $B = \partial_{yy}$ in the square domain $\Omega = (0, 1)^2$ with homogeneous Dirichlet boundary conditions, and $v(x, y) = (16x(1-x)y(1-y))^p$, for $p = 0, 1, 2, 3$. Then, we clearly see in Figure 1.1 that the decay rate of the local error in the approximation of $u(\tau)$ is three (as expected) only for $p = 3$, it drops to two for $p = 2$ or $p = 1$ and to one for $p = 0$. The phenomenon of order reduction in the numerical solution of time-dependent initial boundary value problems is well-known in the literature, in particular in the context of splitting methods [2, 3, 11, 12] and Lawson schemes [1, 8]. Here, however, we are interested in investigating *split exponential integrators* built on splitting approximations of the φ_1 and high-order φ functions in the presence of terms that may not satisfy boundary conditions. In particular, in section 2 we study the local error of the approximations using the abstract framework of strongly continuous commuting semigroups. The analysis is carried out for the case of two operators, but it easily extends to more operators. We also present numerical experiments that verify the theoretical findings. Then, in section 3, we consider two split versions (denoted ERK2L and ERK2) of ETD2RK, a popular second-order

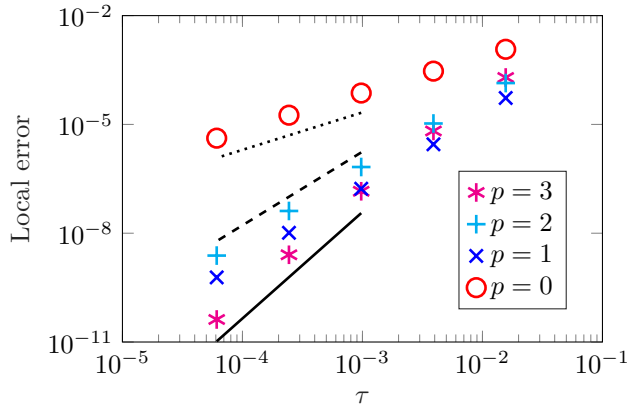


FIG. 1.1. Observed decay rate of the local error $\|u_1 - u(\tau)\|_\infty$ (see formula (1.6)) for the function $v(x, y) = (16x(1-x)y(1-y))^p$, with $p = 0, 1, 2, 3$. The spatial discretization is performed with 250^2 interior points and standard second-order finite differences. The slope of the dotted line is one, that of the dashed line is two, and that of the solid line is three.

exponential integrator of the Runge–Kutta type. We show that, under appropriate assumptions, in our cases of interest ERK2L can have order reduction down to one, while ERK2 is always second-order convergent (in the stiff sense). We demonstrate this with some numerical examples in two and three spatial dimensions. Finally, we draw the conclusions and present possible further developments in section 4.

2. Splitting of φ functions. As mentioned in the introduction, we perform our analysis in an abstract framework, i.e., we consider the abstract ordinary differential equation

$$(2.1) \quad \begin{cases} u'(t) = (A + B)u(t) + g(u(t)) = f(u(t)), \\ u(0) = u_0, \end{cases}$$

associated to the partial differential equation (1.1). A reader not familiar with this formalism is invited to consult for example [14, 21, 23]. In this section we make the following assumptions.

Assumption 2.1. Let X be a Banach space with norm $\|\cdot\|$, and let $A: \mathcal{D}(A) \subset X \rightarrow X$ and $B: \mathcal{D}(B) \subset X \rightarrow X$ be linear operators. We assume that A and B generate strongly continuous semigroups $\{e^{tA}\}_{t \geq 0}$ and $\{e^{tB}\}_{t \geq 0}$.

Assumption 2.2. We assume that the operators A and B commute in the sense of the semigroups, i.e., $e^{tA}e^{tB} = e^{tB}e^{tA}$.

Under Assumptions 2.1 and 2.2 we have that $e^{tA}e^{tB}$ is a strongly continuous semigroup with generator $\overline{A+B}$: $\mathcal{D}(A+B) = \mathcal{D}(A) \cap \mathcal{D}(B) \subset X \rightarrow X$ [14, 25], i.e.,

$$(2.2) \quad e^{tA}e^{tB} = e^{t(A+B)}.$$

Note that in our cases of interest $A+B$ is a closed operator, and therefore we omit the closure from the notation. Furthermore, the following bound

$$(2.3) \quad \|e^{tA}\| \leq C, \quad 0 \leq t \leq T,$$

holds for the operator A (and analogously for the operators B and $A + B$). Here and throughout the paper C denotes a generic constant that can have different values at different occurrences, but it is independent of the stiffness of the problem. Thanks to the bound (2.3), we get that the φ_ℓ functions appearing in exponential integrators, defined by

$$(2.4) \quad \varphi_0(z) = e^z, \quad \varphi_\ell(z) = \frac{1}{(\ell-1)!} \int_0^1 \theta^{\ell-1} e^{(1-\theta)z} d\theta = \sum_{k=0}^{\infty} \frac{z^k}{(\ell+k)!}, \quad \ell > 0$$

satisfy $\|\varphi_\ell(tA)\| \leq C$ for $0 \leq t \leq T$. Also, from their definition it easily follows that the recursive formula

$$(2.5) \quad \varphi_\ell(z) = \frac{\varphi_{\ell-1}(z) - \varphi_{\ell-1}(0)}{z}, \quad \ell > 0$$

holds true. Finally, we note that we present here the analysis for two operators only (for simplicity of exposition). The generalization to more than two operators is straightforward; see Remark 2.11.

2.1. Splitting of φ_1 . We start the analysis with the split approximation of $\tau\varphi_1(\tau(A+B))$ mentioned in the introduction (see formula (1.6)), i.e.,

$$(2.6) \quad \tau\varphi_1(\tau(A+B)) \approx \tau e^{\frac{\tau}{2}A} \varphi_1(\tau B).$$

Note that for *bounded operators* A and B it follows by standard Taylor expansion that

$$\tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}A} \varphi_1(\tau B) = \frac{\tau^3}{24} (A^2 + 2BA) + \mathcal{O}(\tau^4).$$

For unbounded operators, these identities require the function to which they are applied to be sufficiently smooth. In the following lemmas, all operators act on sufficiently regular functions without further mention. The exact regularity assumptions are discussed in the corresponding propositions.

LEMMA 2.3. *Under Assumptions 2.1 and 2.2 we have*

$$\begin{aligned} \tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}A} \varphi_1(\tau B) = & - \int_0^\tau \int_0^s \left(\frac{\tau}{2} - s \right) e^{\tau A} e^{(\tau-\xi)B} B A d\xi ds \\ & - \int_0^\tau \int_s^{\frac{\tau}{2}} \int_0^\sigma e^{(\tau-s)B} e^{(\tau-\xi)A} A^2 d\xi d\sigma ds. \end{aligned}$$

Proof. From the integral representation of the φ_1 function (see (2.4)) we have

$$(2.7) \quad \tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}A} \varphi_1(\tau B) = \int_0^\tau \left(e^{(\tau-s)(A+B)} - e^{\frac{\tau}{2}A} e^{(\tau-s)B} \right) ds.$$

By using the commutativity of the semigroups and inserting

$$(2.8) \quad e^{\frac{\tau}{2}A} = e^{(\tau-s)A} - \int_s^{\frac{\tau}{2}} e^{(\tau-\sigma)A} A d\sigma$$

into the right-hand side, we get

$$(2.9) \quad \tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}A} \varphi_1(\tau B) = \int_0^\tau \int_s^{\frac{\tau}{2}} e^{(\tau-s)B} e^{(\tau-\sigma)A} A d\sigma ds.$$

Now, by substituting

$$(2.10) \quad e^{(\tau-\sigma)A} = e^{\tau A} - \int_0^\sigma e^{(\tau-\xi)A} A d\xi,$$

the right-hand side of (2.9) becomes

$$\int_0^\tau \int_s^{\frac{\tau}{2}} e^{(\tau-s)B} e^{\tau A} A d\sigma ds - \int_0^\tau \int_s^{\frac{\tau}{2}} \int_0^\sigma e^{(\tau-s)B} e^{(\tau-\xi)A} A^2 d\xi d\sigma ds.$$

The second term is in the form given in the statement. Concerning the first term, integrating with respect to σ we have

$$\int_0^\tau \int_s^{\frac{\tau}{2}} e^{(\tau-s)B} e^{\tau A} A d\sigma ds = \int_0^\tau \left(\frac{\tau}{2} - s\right) e^{(\tau-s)B} e^{\tau A} A ds = \int_0^\tau \left(\frac{\tau}{2} - s\right) e^{\tau A} e^{(\tau-s)B} A ds.$$

Let us consider now (2.10) with s and B instead of σ and A , respectively. If we insert it in the right-hand side above, we get

$$\int_0^\tau \left(\frac{\tau}{2} - s\right) e^{\tau A} e^{(\tau-s)B} A ds = - \int_0^\tau \int_0^s \left(\frac{\tau}{2} - s\right) e^{\tau A} e^{(\tau-\xi)B} B A d\xi ds,$$

where we used the fact that

$$\int_0^\tau \left(\frac{\tau}{2} - s\right) ds = 0.$$

This concludes the proof. $\square$

PROPOSITION 2.4. *Let Assumptions 2.1 and 2.2 be valid. Then, the following bounds on the local error*

$$\lambda_1 = \|\tau\varphi_1(\tau(A+B))v - \tau e^{\frac{\tau}{2}A}\varphi_1(\tau B)v\|$$

hold:

- (a) if $v \in \mathcal{D}(A^2) \cap \mathcal{D}(BA)$, then $\lambda_1 \leq C\tau^3$;
- (b) if $v \in \mathcal{D}(A)$, then $\lambda_1 \leq C\tau^2$;
- (c) if $v \notin \mathcal{D}(A)$, then $\lambda_1 \leq C\tau$.

Proof. The first statement follows directly from Lemma 2.3 and the bounds on the semigroups generated by A and B ; see (2.3). For the second statement, we note that the argument below (2.9) cannot be made, and therefore we obtain the result by bounding (2.9) using the estimate (2.3) on the semigroups. For the third statement, similarly to the previous case, we stop at (2.7) and we obtain the desired result. $\square$

Note that, in our cases of interest, the order reduction occurs because the boundary conditions are not satisfied, and *not* because of the lack of spatial regularity of the functions. This means, for example, that a sufficiently smooth function v satisfies statement (a) in Proposition 2.4 if v satisfies the boundary conditions of A and B , and in addition Av satisfies the boundary conditions of A (see subsection 2.3 for some numerical examples).

We observe that the approximation (2.6) is not symmetric with respect to the operators A and B . In fact, if we interchange them, we obtain a different approximation with results (a)–(c) in Proposition 2.4 modified accordingly. A symmetric approximation is

$$(2.11) \quad \tau\varphi_1(\tau(A+B)) \approx \tau e^{\frac{\tau}{2}A} e^{\frac{\tau}{2}B} = \tau e^{\frac{\tau}{2}(A+B)}.$$

Again, in the case of bounded operators A and B , we have by Taylor expansion that

$$\tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}(A+B)} = \frac{\tau^3}{24}(A+B)^2 + \mathcal{O}(\tau^4).$$

LEMMA 2.5. *Under Assumptions 2.1 and 2.2 we have*

$$\begin{aligned} \tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}(A+B)} &= \int_0^\tau \int_0^s \int_{\frac{\tau}{2}}^\sigma e^{(\tau-\xi)(A+B)} (A+B)^2 d\xi d\sigma ds \\ &\quad + \frac{\tau^3}{4} e^{\frac{\tau}{2}(A+B)} \varphi_2\left(\frac{\tau}{2}(A+B)\right) (A+B)^2. \end{aligned}$$

Proof. Similarly to the proof of Lemma 2.3, from the integral representation of the φ_1 function (2.4) we have

$$(2.12) \quad \tau\varphi_1(\tau(A+B)) - \tau e^{\frac{\tau}{2}(A+B)} = \int_0^\tau \left(e^{(\tau-s)(A+B)} - e^{\frac{\tau}{2}(A+B)} \right) ds.$$

Then, by exploiting (2.10) with s and $A+B$ instead of σ and A , respectively, the right-hand side becomes

$$\int_0^\tau \left(e^{\tau(A+B)} - \int_0^s e^{(\tau-\sigma)(A+B)} (A+B) d\sigma - e^{\frac{\tau}{2}(A+B)} \right) ds.$$

We equivalently write this expression as

$$(2.13) \quad - \int_0^\tau \int_0^s e^{(\tau-\sigma)(A+B)} (A+B) d\sigma ds + \frac{\tau^2}{2} e^{\frac{\tau}{2}(A+B)} \varphi_1\left(\frac{\tau}{2}(A+B)\right) (A+B),$$

where we employed the recursive formula for the φ_1 function (2.5). Inserting (2.8) with σ and $A+B$ instead of s and A , respectively, into the integral term we get

$$\int_0^\tau \int_0^s \int_{\frac{\tau}{2}}^\sigma e^{(\tau-\xi)(A+B)} (A+B)^2 d\xi d\sigma ds + \frac{\tau^3}{4} e^{\frac{\tau}{2}(A+B)} \varphi_2\left(\frac{\tau}{2}(A+B)\right) (A+B)^2,$$

where we exploited the recursive formula for the φ_2 function (see again (2.5)). This concludes the proof. $\square$

PROPOSITION 2.6. *Let Assumptions 2.1 and 2.2 be valid. Then, the following bounds on the local error*

$$\lambda_2 = \|\tau\varphi_1(\tau(A+B))v - \tau e^{\frac{\tau}{2}(A+B)}v\|$$

hold:

- (a) if $v \in \mathcal{D}((A+B)^2)$, then $\lambda_2 \leq C\tau^3$;
- (b) if $v \in \mathcal{D}(A+B)$, then $\lambda_2 \leq C\tau^2$;
- (c) if $v \notin \mathcal{D}(A+B)$, then $\lambda_2 \leq C\tau$.

Proof. Using arguments similar to the proof of Proposition 2.4, exploiting the bounds on the semigroup and on the φ_2 function, the first statement follows directly from Lemma 2.5, while the second and the third statements follow from (2.13) and (2.12), respectively. $\square$

We finally consider the symmetric approximation

$$(2.14) \quad \tau\varphi_1(\tau(A+B)) \approx \tau\varphi_1(\tau A)\varphi_1(\tau B).$$

This is actually the approximation already employed in [5]. By Taylor expansion, in the case of commuting bounded operators, we have

$$\tau\varphi_1(\tau(A+B)) - \tau\varphi_1(\tau A)\varphi_1(\tau B) = \frac{\tau^3}{12}BA + \mathcal{O}(\tau^4).$$

We can then prove the following.

LEMMA 2.7. *Under Assumptions 2.1 and 2.2 we have*

$$\begin{aligned} & \tau\varphi_1(\tau(A+B)) - \tau\varphi_1(\tau A)\varphi_1(\tau B) \\ &= \frac{1}{\tau} \int_0^\tau \int_0^\tau \int_s^\sigma (\tau-s)e^{(\tau-\xi)A} \varphi_1((\tau-s)B) B A d\xi d\sigma ds. \end{aligned}$$

Proof. From the integral definition of the φ_1 function (2.4), and using the commutativity of the semigroups, we have

$$\begin{aligned} (2.15) \quad \tau\varphi_1(\tau(A+B)) - \tau\varphi_1(\tau A)\varphi_1(\tau B) &= \int_0^\tau e^{(\tau-s)(A+B)} ds \\ &\quad - \frac{1}{\tau} \int_0^\tau e^{(\tau-s)B} \left(\int_0^\tau e^{(\tau-\sigma)A} d\sigma \right) ds. \end{aligned}$$

Now, by using the fact that

$$e^{(\tau-\sigma)A} = e^{(\tau-s)A} - \int_s^\sigma e^{(\tau-\xi)A} A d\xi,$$

the right-hand side becomes

$$\int_0^\tau e^{(\tau-s)(A+B)} ds - \int_0^\tau e^{(\tau-s)B} \left(e^{(\tau-s)A} - \frac{1}{\tau} \int_0^\tau \int_s^\sigma e^{(\tau-\xi)A} A d\xi d\sigma \right) ds.$$

Exploiting (2.2), we then get

$$(2.16) \quad \tau\varphi_1(\tau(A+B)) - \tau\varphi_1(\tau A)\varphi_1(\tau B) = \frac{1}{\tau} \int_0^\tau \int_0^\tau \int_s^\sigma e^{(\tau-s)B} e^{(\tau-\xi)A} A d\xi d\sigma ds.$$

Finally, by using the commutativity of the semigroups, the right-hand side can be equivalently written as

$$\begin{aligned} \frac{1}{\tau} \int_0^\tau \int_0^\tau \int_s^\sigma e^{(\tau-\xi)A} e^{(\tau-s)B} A d\xi d\sigma ds &= \frac{1}{\tau} \int_0^\tau \int_0^\tau \int_s^\sigma e^{(\tau-\xi)A} (e^{(\tau-s)B} - I) A d\xi d\sigma ds \\ &= \frac{1}{\tau} \int_0^\tau \int_0^\tau \int_s^\sigma (\tau-s) e^{(\tau-\xi)A} \varphi_1((\tau-s)B) B A d\xi d\sigma ds. \end{aligned}$$

Here, we also exploited that

$$\int_0^\tau \int_0^\tau \int_s^\sigma e^{(\tau-\xi)A} A d\xi d\sigma ds = \int_0^\tau \int_0^\tau (e^{(\tau-s)A} - e^{(\tau-\sigma)A}) d\sigma ds = 0$$

and the recursive definition of the φ_1 function (2.5). This concludes the proof. $\square$

PROPOSITION 2.8. *Let Assumptions 2.1 and 2.2 be valid. Then, the following bounds on the local error*

$$\lambda_3 = \|\tau\varphi_1(\tau(A+B))v - \tau\varphi_1(\tau A)\varphi_1(\tau B)v\|$$

hold:

- (a) if $v \in \mathcal{D}(BA)$, then $\lambda_3 \leq C\tau^3$;
- (b) if $v \in \mathcal{D}(A)$, then $\lambda_3 \leq C\tau^2$;
- (c) if $v \notin \mathcal{D}(A)$, then $\lambda_3 \leq C\tau$.

Proof. The first statement follows directly from Lemma 2.7, using the bounds on the semigroup and on the φ_1 function. As in the previous propositions, the second and the third statement follow from intermediate results, in this case (2.16) and (2.15), respectively. $\square$

Note that in (2.14) we can interchange arbitrarily the operators A and B , since it is a symmetric approximation. Therefore, statements similar to (a)–(c) in Proposition 2.8 in terms of $\mathcal{D}(AB)$ and $\mathcal{D}(B)$ hold true.

2.2. Splitting of φ_ℓ . We consider here the general symmetric approximation

$$(2.17) \quad \tau\varphi_\ell(\tau(A+B)) \approx \ell! \tau\varphi_\ell(\tau A)\varphi_\ell(\tau B),$$

which was already employed in [5].

LEMMA 2.9. *Under Assumptions 2.1 and 2.2 we have*

$$\begin{aligned} & \tau\varphi_\ell(\tau(A+B)) - \ell! \tau\varphi_\ell(\tau A)\varphi_\ell(\tau B) \\ &= \frac{\ell}{\tau^{2\ell-1}(\ell-1)!} \int_0^\tau \int_0^\tau \int_s^\sigma (\sigma s)^{(\ell-1)} (\tau-s) e^{(\tau-s)A} \varphi_1((\tau-s)B) B A d\xi d\sigma ds. \end{aligned}$$

Proof. From the integral definition of the φ_ℓ function (2.4), using the commutativity of the semigroups, we have

$$\begin{aligned} \tau\varphi_\ell(\tau(A+B)) - \ell! \tau\varphi_\ell(\tau A)\varphi_\ell(\tau B) &= \frac{1}{\tau^{\ell-1}(\ell-1)!} \int_0^\tau s^{\ell-1} e^{(\tau-s)(A+B)} ds \\ &\quad - \frac{\ell}{\tau^{2\ell-1}(\ell-1)!} \int_0^\tau s^{\ell-1} e^{(\tau-s)B} \left(\int_0^\tau \sigma^{\ell-1} e^{(\tau-\sigma)A} d\sigma \right) ds. \end{aligned}$$

Taking into account that

$$\int_0^\tau \int_0^\tau (\sigma s)^{\ell-1} \left(e^{(\tau-s)A} - e^{(\tau-\sigma)A} \right) d\sigma ds = 0,$$

the proof follows along the steps of Lemma 2.7. $\square$

For the split exponential integrators that we will consider in section 3 we need local error bounds for the φ_2 function. Therefore, we state the following proposition just for the case $\ell = 2$.

PROPOSITION 2.10. *Let Assumptions 2.1 and 2.2 be valid. Then, the following bounds on the local error*

$$\lambda_4 = \|\tau\varphi_2(\tau(A+B))v - 2\tau\varphi_2(\tau A)\varphi_2(\tau B)v\|$$

hold:

- (a) if $v \in \mathcal{D}(BA)$, then $\lambda_4 \leq C\tau^3$;
- (b) if $v \in \mathcal{D}(A)$, then $\lambda_4 \leq C\tau^2$;
- (c) if $v \notin \mathcal{D}(A)$, then $\lambda_4 \leq C\tau$.

Proof. The result follows from Lemma 2.9 and reasoning similar to that in Proposition 2.8. $\square$

Remark 2.11. As mentioned at the beginning of the section, we fully developed the analysis for the case of two commuting operators. The case with d operators follows straightforwardly. In fact, we have (see also [5])

$$\|\tau\varphi_\ell(\tau(A_1 + \cdots + A_d))v - (\ell!)^{d-1} \tau\varphi_\ell(\tau A_1) \cdots \varphi_\ell(\tau A_d)v\| \leq C\tau^3$$

TABLE 2.1

Summary of the functions $v = v(x, y)$ and of the split approximations to $\tau\varphi_1(\tau(A + B))v$ and $\tau\varphi_2(\tau(A + B))v$ (see (2.6), (2.11), (2.14), and (2.17)) employed in the numerical experiments of subsection 2.3. Here $A = \partial_{xx}$, $B = \partial_{yy}$ (with homogeneous Dirichlet boundary conditions), and $X = C((0, 1)^2)$.

$v = v(x, y)$	$\mathcal{D}(A)$	$\mathcal{D}(A^2)$	$\mathcal{D}(BA)$	$\mathcal{D}(A + B)$	$\mathcal{D}((A + B)^2)$
$v_1 = 4^6(x(1-x)y(1-y))^3$	✓	✓	✓	✓	✓
$v_2 = 4^4(x(1-x))^3y(1-y)$	✓	✓	✓	✓	×
$v_3 = 4^2x(1-x)y(1-y)$	✓	×	✓	✓	×
$v_4 = 4x(1-x)$	✓	×	×	×	×
$v_5 = 1$	×	×	×	×	×

(a) Functions $v = v(x, y)$.

v	$\tau e^{\frac{\tau}{2}A}\varphi_1(\tau B)v$	$\tau e^{\frac{\tau}{2}A}e^{\frac{\tau}{2}B}v$	$\tau\varphi_1(\tau A)\varphi_1(\tau B)v$	$2\tau\varphi_2(\tau A)\varphi_2(\tau B)v$
v_1	3	3	3	3
v_2	3	2	3	3
v_3	2	2	3	3
v_4	2	1	2	2
v_5	1	1	1	1

(b) Expected decay rates of the local errors.

if v is a sufficiently smooth function that satisfies the boundary conditions of the operators $A_1, \dots, A_d$. If not, we encounter similar order reductions as for the case of two operators.

2.3. Numerical experiments on the split approximations. In the following experiments we compare the split approximations to $\tau\varphi_1(\tau(A + B))v$ and $\tau\varphi_2(\tau(A + B))v$ introduced in the previous sections. To this aim, we consider the space of continuous functions $X = C(\Omega)$, equipped with the infinity norm, on the square domain $\Omega = (0, 1)^2$. The operators are $A = \partial_{xx}$ and $B = \partial_{yy}$ with homogeneous Dirichlet boundary conditions. We consider smooth functions $v = v(x, y)$ such that their partial derivatives satisfy or not the boundary conditions. The operators are approximated by standard second-order finite differences (with 250^2 interior discretization points). We consider a common range of time step sizes τ and measure the decay rate of the local error for the different approximations. The selected functions v are presented in Table 2.1a. In Table 2.1b we collect the expected decay rates of the local errors, according to the results obtained in the previous sections. The numerical results, summarized in Figure 2.1, match satisfactorily the theoretical findings.

3. Convergence analysis of two split versions of ETD2RK. In this section, we apply the local error bounds that we have found in section 2 to show the convergence (in the stiff sense) of two split versions of a popular second-order exponential Runge–Kutta integrator, also known in the literature as ETD2RK. To this aim, we consider the abstract evolution equation (2.1), for which the integrator can be written as [17, Tableau 5.3, $c_2 = 1$]

$$(3.1a) \quad \begin{aligned} \tilde{U}_{n2} &= e^{\tau(A+B)}\tilde{u}_n + \tau\varphi_1(\tau(A+B))g(\tilde{u}_n) \\ \tilde{u}_{n+1} &= \tilde{U}_{n2} + \tau\varphi_2(\tau(A+B))(g(\tilde{U}_{n2}) - g(\tilde{u}_n)), \end{aligned}$$

or equivalently as

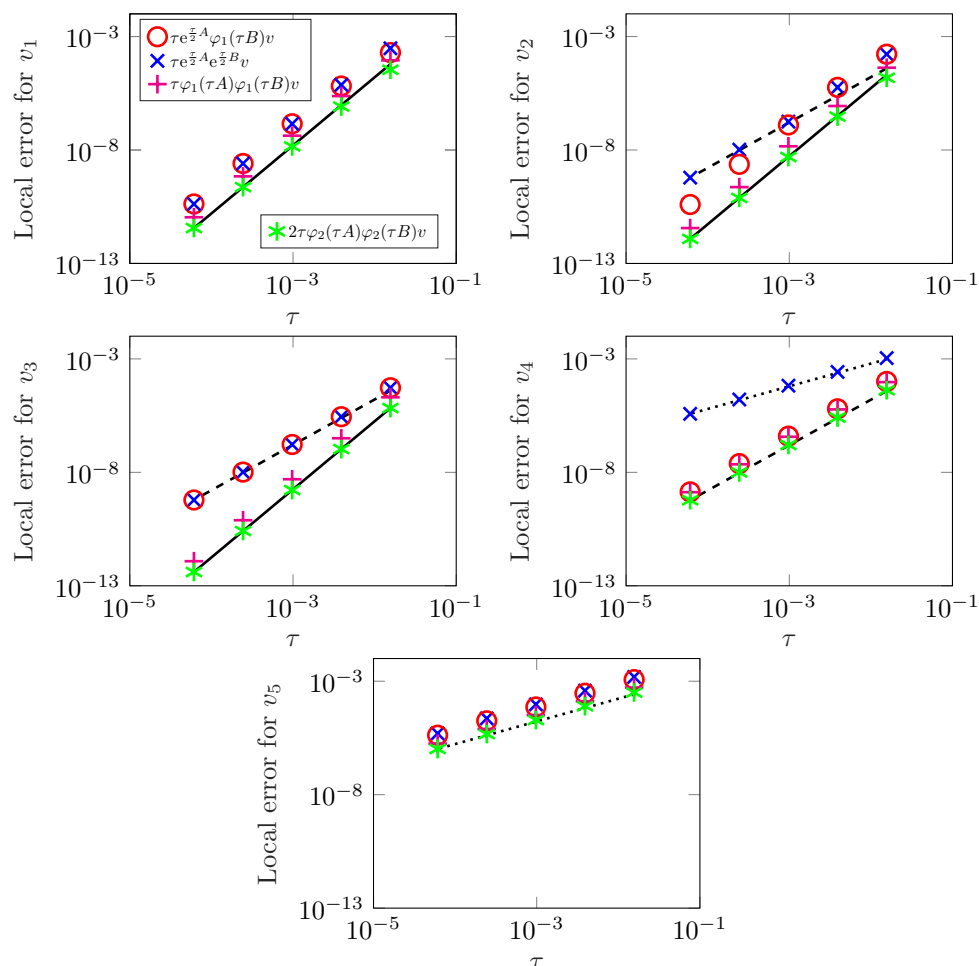


FIG. 2.1. Observed decay rates of the local errors (in the infinity norm) of the split approximations to $\tau \varphi_1(\tau(A+B))v$ and $\tau \varphi_2(\tau(A+B))v$ for the different functions $v = v(x, y)$; see Table 2.1. The slope of the dotted line is one, that of the dashed line is two, and that of the solid line is three.

$$(3.1b) \quad \begin{aligned} \tilde{U}_{n2} &= \tilde{u}_n + \tau \varphi_1(\tau(A+B))f(\tilde{u}_n), \\ \tilde{u}_{n+1} &= \tilde{U}_{n2} + \tau \varphi_2(\tau(A+B))(g(\tilde{U}_{n2}) - g(\tilde{u}_n)). \end{aligned}$$

Here $\tilde{u}_n \approx u(t_n)$, with $t_n = n\tau$ and $\tau = T/N$ (N is the total number of time steps). To study the global error we make the following assumptions.

Assumption 3.1. Let X be a Banach space with norm $\|\cdot\|$. Let $A: \mathcal{D}(A) \subset X \rightarrow X$ and $B: \mathcal{D}(B) \subset X \rightarrow X$ be linear operators. We assume that A , B and $A+B$ generate analytic semigroups $\{e^{tA}\}_{t \geq 0}$, $\{e^{tB}\}_{t \geq 0}$ and $\{e^{t(A+B)}\}_{t \geq 0}$.

Note that Assumption 3.1 implies that the *parabolic smoothing* bound

$$\|(-tA)^\alpha e^{tA}\| \leq C, \quad \alpha > 0, \quad t \in [0, T]$$

holds (similarly for the operators B and $A+B$).

Assumption 3.2. We assume that equation (2.1) possesses a sufficiently smooth solution $u: [0, T] \rightarrow X$ with derivatives in X and that $g: X \rightarrow X$ is twice Fréchet differentiable, with uniformly bounded derivatives. This in particular implies that g is a Lipschitz function.

3.1. Split exponential integrator ERK2L. We start by considering the following split version of integrator (3.1a)

$$(3.2) \quad \begin{aligned} U_{n2} &= e^{\tau A} e^{\tau B} u_n + \tau \varphi_1(\tau A) \varphi_1(\tau B) g(u_n), \\ u_{n+1} &= U_{n2} + 2\tau \varphi_2(\tau A) \varphi_2(\tau B) (g(U_{n2}) - g(u_n)), \end{aligned}$$

that we call ERK2L. The same idea was employed in [4, Formula 22] to obtain a directional split version of the exponential Euler method. Notice that integrator (3.2) is exact for *linear* homogeneous problems (that is, $g \equiv 0$).

THEOREM 3.3. *Let Assumptions 2.2, 3.1, and 3.2 be valid. Then, the following bounds on the global error of scheme (3.2), i.e.,*

$$e_{n,L} = \|u_n - u(t_n)\|, \quad 0 \leq n\tau \leq T,$$

hold:

- (a) *if $g(u(t)) \in \mathcal{D}(BA)$, then $e_{n,L} \leq C\tau^2$;*
 - (b) *if $g(u(t)) \in \mathcal{D}(A)$, then $e_{n,L} \leq C\tau^2(1 + |\log \tau|)$;*
 - (c) *if $g(u(t)) \notin \mathcal{D}(A)$, then $e_{n,L} \leq C\tau$.*
- The constant C is independent of n and τ , but it depends on T .*

Proof. Let $h(t) = g(u(t))$. We consider the variation-of-constants formula (1.2) with $t = t_{n+1}$ and the Taylor expansion

$$(3.3) \quad h(t_n + s) = h(t_n) + h'(t_n)s + \int_0^s (s - \sigma)h''(t_n + \sigma)d\sigma.$$

Then, for the stage U_{n2} (which approximates $u(t_n + \tau) = u(t_{n+1})$) we have

$$U_{n2} - u(t_{n+1}) = e^{\tau(A+B)} \epsilon_n + \sum_{i=1}^4 \rho_{n,i},$$

where

$$\begin{aligned} \epsilon_n &= u_n - u(t_n), \\ \rho_{n,1} &= \tau(\varphi_1(\tau A)\varphi_1(\tau B) - \varphi_1(\tau(A+B)))h(t_n), \\ \rho_{n,2} &= \tau\varphi_1(\tau A)\varphi_1(\tau B)(g(u_n) - h(t_n)), \\ \rho_{n,3} &= -\tau^2\varphi_2(\tau(A+B))h'(t_n), \\ \rho_{n,4} &= -\int_0^\tau e^{(\tau-s)(A+B)} \int_0^s (s - \sigma)h''(t_n + \sigma)d\sigma ds. \end{aligned}$$

Note that $\rho_{n,1}$ satisfies

$$\|\rho_{n,1}\| \leq C\tau^\alpha \quad \text{with} \quad \alpha = \begin{cases} 3 & \text{if } h(t_n) \in \mathcal{D}(BA) \\ 2 & \text{if } h(t_n) \in \mathcal{D}(A) \\ 1 & \text{if } h(t_n) \notin \mathcal{D}(A) \end{cases}$$

thanks to Proposition 2.8. Also, $\|\rho_{n,2}\| \leq C\tau\|\epsilon_n\|$ (since g is Lipschitz) and $\|\rho_{n,4}\| \leq C\tau^3$. Then, for estimating the global error

$$\epsilon_{n+1} = u_{n+1} - u(t_{n+1}) = U_{n2} - u(t_{n+1}) + 2\tau\varphi_2(\tau A)\varphi_2(\tau B)(g(U_{n2}) - g(u_n))$$

we need bounds on the last term. To this aim, we write

$$g(U_{n2}) - g(u_n) = (g(U_{n2}) - h(t_{n+1})) + (h(t_n) - g(u_n)) + (h(t_{n+1}) - h(t_n)),$$

thus getting

$$2\tau\varphi_2(\tau A)\varphi_2(\tau B)(g(U_{n2}) - g(u_n)) = \sum_{i=5}^9 \rho_{n,i},$$

where

$$\begin{aligned} \rho_{n,5} &= 2\tau\varphi_2(\tau A)\varphi_2(\tau B)(g(U_{n2}) - h(t_{n+1})), \\ \rho_{n,6} &= 2\tau\varphi_2(\tau A)\varphi_2(\tau B)(h(t_n) - g(u_n)), \\ \rho_{n,7} &= \tau(2\varphi_2(\tau A)\varphi_2(\tau B) - \varphi_2(\tau(A+B)))(h(t_{n+1}) - h(t_n)), \\ \rho_{n,8} &= \tau^2\varphi_2(\tau(A+B))h'(t_n), \\ \rho_{n,9} &= \tau\varphi_2(\tau(A+B)) \int_0^\tau (\tau - \sigma)h''(t_n + \sigma)d\sigma. \end{aligned} \quad (3.4)$$

Here we used again formula (3.3), now with $s = \tau$. Note that, using the fact that g is Lipschitz, the term $\rho_{n,5}$ satisfies $\|\rho_{n,5}\| \leq C\tau\|\epsilon_n\| + C\tau^{\min\{3, \alpha+1\}}$, $\|\rho_{n,6}\| \leq C\tau\|\epsilon_n\|$, $\|\rho_{n,7}\| \leq C\tau^\alpha$ (see Proposition 2.10) and $\|\rho_{n,9}\| \leq C\tau^3$. Therefore, the recursion of the global error is

$$\epsilon_{n+1} = e^{\tau(A+B)}\epsilon_n + \sum_{\substack{i=1 \\ i \neq 3,8}}^9 \rho_{n,i}$$

since $\rho_{n,8} = -\rho_{n,3}$. Then, if $h(t) \in \mathcal{D}(BA)$, we have

$$\|\epsilon_n\| \leq C\tau \sum_{k=1}^{n-1} \|\epsilon_k\| + C\tau^2.$$

Similarly, by exploiting the parabolic smoothing property for the terms related to $\rho_{n,1}$ and $\rho_{n,7}$ we get

$$\|\epsilon_n\| \leq C\tau \sum_{k=1}^{n-1} \|\epsilon_k\| + C\tau^2(1 + |\log \tau|) \quad \text{and} \quad \|\epsilon_n\| \leq C\tau \sum_{k=1}^{n-1} \|\epsilon_k\| + C\tau$$

for the cases $h(t) \in \mathcal{D}(A)$ and $h(t) \notin \mathcal{D}(A)$, respectively. Finally, the application of a discrete Gronwall lemma [18, Lemma 2.15] leads to the result. $\square$

3.2. Split exponential integrator ERK2. We now consider the following split version of integrator (3.1b)

$$\begin{aligned} U_{n2} &= u_n + \tau\varphi_1(\tau A)\varphi_1(\tau B)f(u_n), \\ u_{n+1} &= U_{n2} + 2\tau\varphi_2(\tau A)\varphi_2(\tau B)(g(U_{n2}) - g(u_n)), \end{aligned} \quad (3.5)$$

that we call ERK2. This is the directional split exponential integrator employed, e.g., in [5]. We start by studying the linear stability of scheme (3.5), i.e., the stability of the recursion

$$u_{n+1} = R(\tau A, \tau B)u_n$$

with

$$R(\tau A, \tau B) = I + \tau \varphi_1(\tau A) \varphi_1(\tau B)(A + B).$$

To avoid the intricacies of functional analysis, we make the following assumptions.

Assumption 3.4. We assume that there exists a bounded operator V , with bounded inverse, such that the commuting operators A and B satisfy

$$A = V^{-1} M_{q_A} V \quad \text{and} \quad B = V^{-1} M_{q_B} V.$$

Here, M_{q_A} and M_{q_B} denote multiplication operators with functions q_A and q_B having values in $(-\infty, 0]$.

Note that, since A and B commute, they are transformed by the same operator V .

Assumption 3.5. Let M_q be a multiplication operator. We assume that

$$\|M_q\| \leq \|q\|_\infty.$$

Note that this is in fact an equality, e.g., in the space of continuous functions and in L^p spaces; see [14].

LEMMA 3.6. *Let Assumptions 3.4 and 3.5 be valid. Then, we have*

$$(3.6) \quad \|R(\tau A, \tau B)^n\| \leq C$$

for $0 \leq n\tau \leq T$.

Proof. The result follows easily from the estimate

$$\|R(\tau A, \tau B)^n\| \leq \|V^{-1}\| \|V\| \|R(\tau M_{q_A}, \tau M_{q_B})\|^n$$

and the fact that $|R(a, b)| \leq 1$ for $a, b \leq 0$. □

We are now in a position to prove the following result.

THEOREM 3.7. *Let Assumptions 2.2, 3.1, 3.2, 3.4, and 3.5 be valid. Furthermore, assume that $g(u(t)) - g(u(s)) \in \mathcal{D}(BA)$ for all $0 \leq t, s \leq T$. Then, the following bound on the global error of scheme (3.5) holds:*

$$e_n = \|u_n - u(t_n)\| \leq C\tau^2, \quad 0 \leq n\tau \leq T.$$

The constant C is independent of n and τ , but it depends on T .

Proof. The proof is very similar to that of Theorem 3.3. Setting $h(t) = g(u(t))$, and exploiting the variation-of-constants formula with $t = t_{n+1}$, we get for the stage

$$\begin{aligned} U_{n2} - u(t_{n+1}) &= R(\tau A, \tau B)(u_n - u(t_n)) \\ &\quad + \tau(\varphi_1(\tau A)\varphi_1(\tau B) - \varphi_1(\tau(A+B)))f(u(t_n)) \\ &\quad + \tau\varphi_1(\tau A)\varphi_1(\tau B)(g(u_n) - h(t_n)) \\ &\quad - \int_0^\tau e^{\tau(A+B)}(h(t_n+s) - h(t_n))ds. \end{aligned}$$

The second term is bounded by $C\tau^3$, since $f(u(t)) \in \mathcal{D}(BA)$ (it always satisfies the boundary conditions as $u'(t) = f(u(t))$ does). For the remaining terms and the rest

of the proof, employing the Taylor expansion (3.3) and the stability bound (3.6) in Lemma 3.6, we proceed as in the proof of Theorem 3.3. Note that, in this case, the term corresponding to $\rho_{n,5}$ (see formula (3.4)) satisfies $\|\rho_{n,5}\| \leq C\tau\|\epsilon_n\| + C\tau^2$, while $\rho_{n,7}$ is always bounded by $C\tau^3$ (as by assumption $h(t) - h(s) \in \mathcal{D}(BA)$). $\square$

Remark 3.8. Although integrators (3.1a) and (3.1b) are equivalent, this is *not* the case for (3.2) and (3.5). In fact, the split scheme (3.2) may have order reduction to one (e.g., if $g(u(t)) \notin \mathcal{D}(A)$), its error constant scales with $g(u(t))$ (see the proof of Theorem 3.3 and the experiments in the next section), and it is exact when $g \equiv 0$. These assertions are not true for the split scheme (3.5) which, on the other hand, in our cases of interest is always second-order accurate (see the numerical experiments in the next section).

3.3. Numerical experiments. In this section, we present some numerical experiments that illustrate the behavior of the two split integrators (3.2) and (3.5) under various circumstances. We perform the experiments using MATLAB R2022a on an Intel Core i7-10750H CPU (equipped with 16 GB of RAM).

We start by considering the following two-dimensional evolution diffusion-reaction equation in the spatial domain $\Omega = (0, 1)^2$

$$(3.7a) \quad \begin{cases} \partial_t u(t, x, y) = \Delta u(t, x, y) + g(u(t, x, y), x, y), \\ u(0, x, y) = 16x(1-x)y(1-y), \end{cases}$$

subject to homogeneous Dirichlet boundary conditions. The nonlinear term is

$$(3.7b) \quad g(u(t, x, y), x, y) = \frac{\kappa q(x, y)^p}{1 + u(t, x, y)^2}, \quad p \in \{0, 1\},$$

with κ a real parameter and $q(x, y) = 16x(1-x)y(1-y)$. Clearly, the nonlinear term *does not* satisfy the boundary conditions if $p = 0$, while it does if $p = 1$. The Laplacian is approximated by standard second-order finite differences with 250^2 interior discretization points. The resulting matrix is $(I \otimes D + D \otimes I)$, where I is the identity matrix, $\otimes$ denotes the Kronecker product, and D is the approximation matrix of the one-dimensional second derivative operator with homogeneous Dirichlet boundary conditions. The actions of the matrix exponentials and the matrix φ functions on a vector v required by the integrators ERK2L and ERK2 are efficiently computed by directionally splitting the discretized Laplacian and exploiting the equivalence

$$\varphi_\ell(\tau(I \otimes D))\varphi_\ell(\tau(D \otimes I))v = (\varphi_\ell(\tau D) \otimes \varphi_\ell(\tau D))v = \text{vec}(\varphi_\ell(\tau D)V\varphi_\ell(\tau D)^T).$$

Here vec denotes the operator which stacks the input matrix by columns and V , on the other hand, is a matrix satisfying $\text{vec}(V) = v$. Note that the realization of the above formula requires only to compute *small* matrix functions (i.e., φ functions of the discretization of the *one-dimensional* second derivative operator) and two dense matrix-matrix products. The matrix functions are computed once and for all before the time integration using a standard Padé approximation with modified scaling and squaring [24]. We compare the integrators with the (unsplit) ETD2RK method (3.1b), in which the required actions of matrix functions $\varphi_\ell(\tau(I \otimes D + D \otimes I))v$ are computed at each time step using the adaptive Krylov subspace solver presented in [15].

The results for $\kappa = 2$ and $\kappa = 0.02$, with final time $T = 0.1$ and number of time steps $N = 2^j$, with $j = 2, 4, 6, 8, 10$, are collected in Figure 3.1. As stated in Theorems 3.3 and 3.7, when the nonlinear term (3.7b) satisfies the boundary conditions

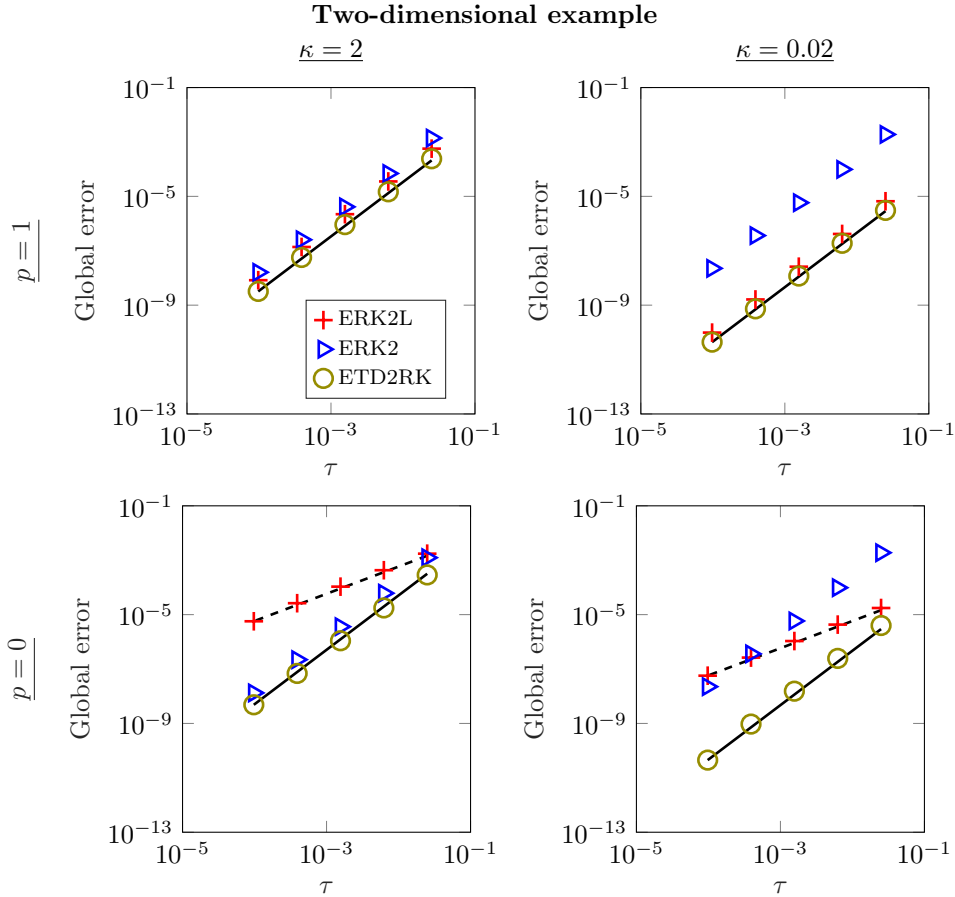


FIG. 3.1. Observed decay rates of the global errors (at $T = 0.1$ in the infinity norm) of ERK2L (3.2), ERK2 (3.5) and ETD2RK (3.1b) for the two-dimensional example (3.7). The slope of the dashed line is one and that of the solid line is two.

($p = 1$, top row in the figure) we observe second-order convergence for both the split schemes. Otherwise ($p = 0$, bottom row), the scheme ERK2L exhibits order reduction to one. Moreover, in contrast to ERK2, we remark that the errors of the schemes ETD2RK and ERK2L scale according to the parameter κ in the nonlinear term. This is expected, since the remainders in the global errors of both schemes are proportional to the nonlinear term (see Remark 3.8). Finally, the average wall-clock time per time step of the split schemes is about 4 milliseconds, while that of the unsplit scheme is roughly 30 milliseconds.

We finally repeat the example in a three-dimensional scenario, i.e., we solve

$$(3.8a) \quad \begin{cases} \partial_t u(t, x, y, z) = \Delta u(t, x, y, z) + g(u(t, x, y, z), x, y, z), \\ u(0, x, y, z) = 64x(1-x)y(1-y)z(1-z), \end{cases}$$

in the spatial domain $\Omega = (0, 1)^3$ with homogeneous Dirichlet boundary conditions. The nonlinear term is

$$(3.8b) \quad g(u(t, x, y, z), x, y, z) = \frac{\kappa q(x, y, z)^p}{1 + u(t, x, y, z)^2}, \quad p \in \{0, 1\},$$

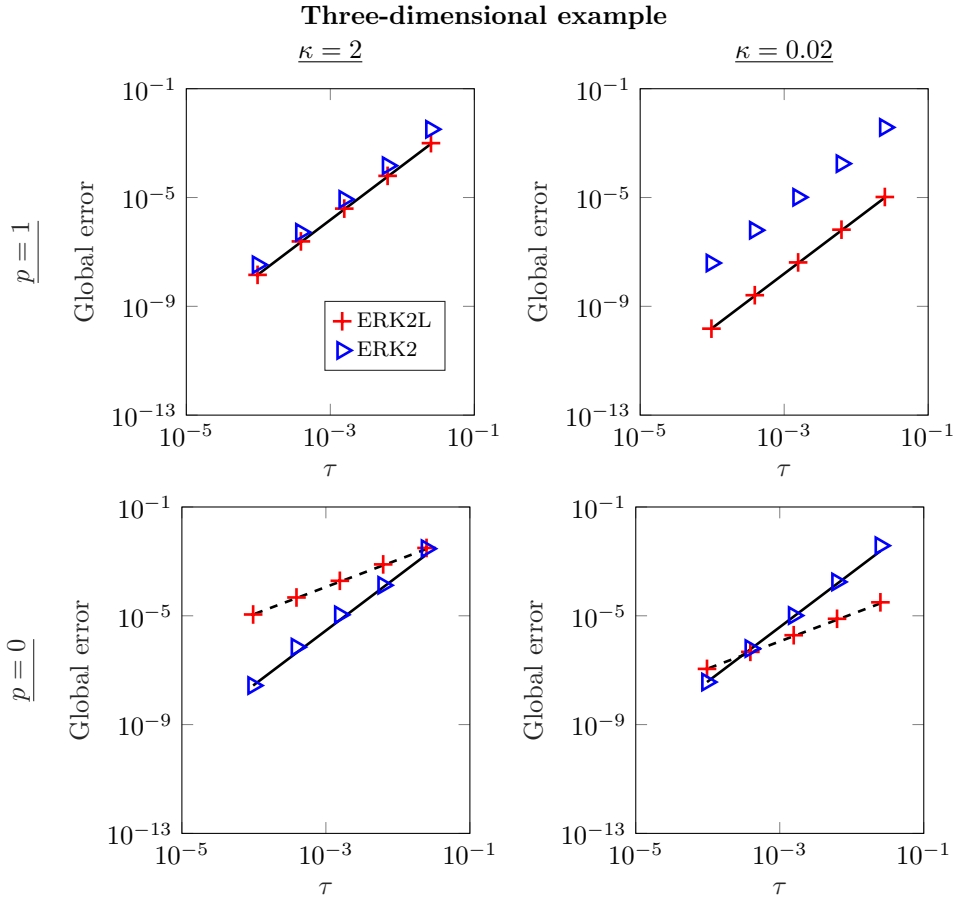


FIG. 3.2. Observed decay rate of the global error (at $T = 0.1$ in the infinity norm) of ERK2L (3.2) and ERK2 (3.5) for the three-dimensional example (3.8). The slope of the dashed line is one and that of the solid line is two.

with $q(x, y, z) = 64x(1 - x)y(1 - y)z(1 - z)$. The Laplacian is approximated by finite differences, this time with 250^3 interior discretization points, resulting in the matrix $(I \otimes I \otimes D + I \otimes D \otimes I + D \otimes I \otimes I)$. In this case, after directional splitting, the action of the matrix functions on a vector v is realized by

$$\begin{aligned} &\varphi_\ell(\tau(I \otimes I \otimes D))\varphi_\ell(\tau(I \otimes D \otimes I))\varphi_\ell(\tau(D \otimes I \otimes I))v \\ &= \text{vec}(V \times_1 \varphi_\ell(\tau D) \times_2 \varphi_\ell(\tau D) \times_3 \varphi_\ell(\tau D)), \end{aligned}$$

where V is an order-3 tensor satisfying $\text{vec}(V) = v$ (here vec is the operator which stacks the input tensor by columns) and $\times_\mu$ denotes the tensor-matrix product along direction μ . Note that the right-hand side is efficiently realized by three dense matrix-matrix products (level 3 BLAS operations). A reader not familiar with the above formalism is invited to consult [5, 6, 7, 9].

From the results collected in Figure 3.2 we draw similar conclusions to that of the two-dimensional case, i.e., the split integrators show the expected behavior and convergence order. In this three-dimensional scenario, the average wall-clock time per time step for the split methods is about 1.4 seconds, while the ETD2RK method

did not finish the computation of the first time step because of too large memory requirements.

4. Conclusions and future work. In this paper, we analyzed split approximations for the φ functions in an abstract setting. In particular, we showed that an order reduction may occur if, for instance, the boundary conditions are not fulfilled by the involved functions. We then employed the derived bounds to prove convergence results for two split versions of a popular second-order exponential integrator for semilinear parabolic equations. The accompanying numerical simulations in two and three spatial dimensions confirm the theoretical results.

An interesting further development is the study of high-order split approximations for φ functions, useful for the effective employment of exponential schemes of order higher than two.

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