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High order splitting methods for analytic semigroups exist

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Abstract In this paper, we are concerned with the construction and analysis of high order exponential splitting methods for the time integration of abstract evolution equations which are evolved by analytic semigroups. We derive a new class of splitting methods of orders three to fourteen based on complex coefficients. An optimal convergence analysis is presented for the methods when applied to equations on Banach spaces with unbounded vector fields. These results resolve the open question whether there exist splitting schemes with convergence rates greater then two in the context of semigroups. As a concrete application we consider parabolic equations and their dimension splittings. The sharpness of our theoretical error bounds is further illustrated by numerical experiments.

Keywords Exponential splitting methods · Analytic semigroups · High order convergence · Parabolic equations

Mathematics Subject Classification (2000) 65M15 · 65J10 · 65L05 · 47D06

1 Introduction

Consider the linear evolution equation

$$\dot{u} = Lu = (A+B)u, \qquad u(0) = u_0, \tag{1.1}$$

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where the unbounded operators L, A and B generate the semigroups e^{tL}, e^{tA} and e^{tB}, respectively. Equations of this form are, for example, found in the context of parabolic problems. A commonly used approach when approximating the solution $u(t) = \mathrm{e}^{tL}u_0$ is to employ an s-stage exponential splitting scheme, i.e., $u(nh) \approx S_h^n u_0$ with

$$S_h = \mathrm{e}^{\gamma_s hA}\mathrm{e}^{\delta_s hB}\ldots\mathrm{e}^{\gamma_1 hA}\mathrm{e}^{\delta_1 hB}. \tag{1.2}$$

The main advantage of these integrators is that they only rely on computations involving the partial flows e^{tA} and e^{tB}, which may tremendously improve the efficiency when compared to integrators based on approximating $\mathrm{e}^{tL}u_0$ directly. Contemporary surveys addressing the usage of exponential splitting methods can be found in [6, 10, 11].

The coefficients γ_j and δ_j in (1.2) are chosen in such a way that the method has *classical* order p, which is achieved by formally expanding S_h and e^{hL} into Taylor series in h and comparing the terms in the expansion up to order p. Our theory, presented in the paper [7], then yields that the splitting method will retain its classical order in the present context of unbounded operators.

It has been a longstanding belief within the numerical analysis community that *it is only possible to apply exponential splitting methods of at most order $p = 2$ to evolution equations which are evolved by semigroups*. This statement is motivated by the fact that splitting schemes with real coefficients γ_j and δ_j necessarily have at least one negative coefficient whenever $p \geq 3$; see [2]. Hence, one can not make use of such schemes here, as the semigroups are not well defined for negative times t. As an illustration, consider the somewhat trivial example of the semigroup $\mathrm{e}^{t\Delta}$ obtained when solving the heat equation $\dot{u} = \Delta u$ on the unit interval with homogeneous Dirichlet boundary conditions. Here, the kth Fourier coefficient of $\mathrm{e}^{t\Delta}u_0$ is of the form $c_k \mathrm{e}^{-(k\pi)^2 t}$ and it is clear that the semigroup is in general not well defined for $t < 0$ in, e.g., $L^2(0,1)$.

What is commonly overlooked is that the statement regarding the order $p = 2$ barrier for splitting schemes only holds true for *real* coefficients γ_j and δ_j, whereas the order conditions yield plenty of schemes of order $p \geq 3$ with complex coefficients in the right half plane of $\mathbb{C}$. Some examples of such splitting schemes are given in the papers [1, 4, 16]. The question is now if one can make sense of the semigroups in this complex valued setting. If we return to the example of the heat equation on the unit interval, it is straightforward to extend $\mathrm{e}^{t\Delta}$ to complex times $t \in \{z \in \mathbb{C} : \mathrm{Re}(z) \geq 0\}$ by using Parseval's equality. In fact, when treating parabolic equations one can always extend the related semigroup into a sector in the right half plane of $\mathbb{C}$, which leads to the theory of *analytic* semigroups. Thus, the aim of this paper is to derive and analyze a new broad class of complex splitting schemes, of order $p \geq 3$ and with coefficients having positive real parts (and small arguments), which can be applied to (1.1).

The paper is organized as follows: We start off in Section 2 by systematically deriving splitting schemes with complex coefficients and of high classical order. Thereafter, in Section 3, we present the needed framework of analytic semigroups and recapitulate the central convergence result. A concrete application of the abstract theory is given in Section 4, where we consider the dimension splitting of parabolic problems. Finally, the theoretical results are illustrated in Section 5, by a wide range of numerical experiments.

2 Derivation of high order splitting schemes with complex coefficients

Our first step is to derive splitting schemes (1.2) of classical order $p \geq 3$ with coefficients γ_j and δ_j in the right half plane of $\mathbb{C}$. There are (at least) two basic strategies to achieve this, either by deriving the schemes from scratch via order conditions, or by constructing them via the composition of lower order splittings. After the submission of the paper, it has come to our attention that the latter approach has also been proposed in the preprint [3]. As a convention, named splittings will be denoted henceforth by capital Greek letters, Φ_h, Ψ_h, etc.

2.1 Deriving schemes from scratch

It is possible to obtain order conditions for an exponential splitting scheme by employing the so called Baker–Campbell–Hausdorff formula; see [6, Section III.5]. For example, the order conditions obtained for an s-stage exponential splitting of order $p = 3$ are

$$c^1_{1,s} = c^1_{2,s} = 1 \qquad \text{and} \qquad c^2_{1,s} = c^3_{1,s} = c^3_{2,s} = 0, \tag{2.1}$$

where the terms $c^k_{\ell,s}$ are given by the recurrence relations

$$\begin{aligned}
c^1_{1,j} &= c^1_{1,j-1} + \delta_j, \qquad c^1_{2,j} = c^1_{2,j-1} + \gamma_j,\\
c^2_{1,j} &= c^2_{1,j-1} + \delta_j\gamma_j + c^1_{1,j-1}\gamma_j - c^1_{2,j-1}\delta_j,\\
c^3_{1,j} &= c^3_{1,j-1} + \delta_j^2\gamma_j + 2c^1_{1,j-1}\delta_j\gamma_j - 3c^2_{1,j-1}\delta_j\\
&\qquad + (c^1_{1,j-1})^2\gamma_j - c^1_{1,j-1}c^1_{2,j-1}\delta_j + c^1_{2,j-1}\delta_j^2,\\
c^3_{2,j} &= c^3_{2,j-1} + \delta_j\gamma_j^2 - 4c^1_{2,j-1}\delta_j\gamma_j + 3c^2_{1,j-1}\gamma_j\\
&\qquad + (c^1_{2,j-1})^2\delta_j - c^1_{1,j-1}c^1_{2,j-1}\gamma_j + c^1_{1,j-1}\gamma_j^2,
\end{aligned}$$

for $j \geq 1$, and $c^k_{\ell,0} = 0$ for all values of k and ℓ. The derivation can be found in connection with the proof of [6, Theorem III.5.6]. For a solution of (2.1), its complex conjugate is again a solution. This follows from the fact that the order conditions are real polynomials. Therefore, we will determine solutions up to conjugation only.

We next discuss how the order conditions (2.1) can be solved with a small number of stages. For $s = 3$, the order conditions consist of five polynomial equations with six unknowns γ_1, γ_2, γ_3, δ_1, δ_2, and δ_3. Generically, a one parameter family solutions exists. For our purpose, it is essential that all method coefficients have positive real parts.

Taking $\delta_2 = \chi$ as free parameter, the order conditions are easily solved in the following way. With the help of the conditions $c^1_{1,s} = c^1_{2,s} = 1$, we express δ_1 by δ_3 and χ, as well as γ_1 by γ_2 and γ_3. We insert these relations into $c^2_{1,s} = 0$ and solve for γ_2. There is a unique solution for $\chi \neq 0$. Next, we insert the so far computed quantities

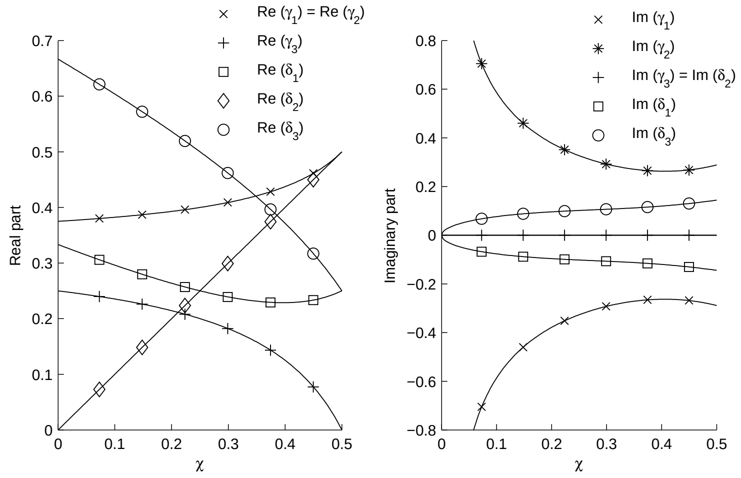

Fig. 2.1 The figures display the real (left) and imaginary (right) parts of the parameter dependent coefficients γ_j and δ_j, which determine the third order exponential splitting family $\Psi_h(\chi)$.

into $c^3_{1,s} = 0$ and solve for γ_3. Again, we get a unique solution for $\chi \neq 0$ and $\chi \neq 3/4$. The condition $c^3_{2,s} = 0$ then becomes a quadratic equation in δ_3 with the solutions

$$\delta_3 = \frac{12 - 27\chi + 12\chi^2 \pm \sqrt{3\chi\left(48\chi^3 - 72\chi^2 + 39\chi - 8\right)}}{18 - 24\chi}. \tag{2.2}$$

Inserting this back gives the sought after family of solutions. For real $\chi \geq 0$, the resulting one parameter family of coefficients is displayed in Figure 2.1. The critical coefficient turns out to be

$$\gamma_3 = \frac{1 - 2\chi}{4 - 6\chi}.$$

To guarantee its admissability, we restrict our attention to the interval $0 < \chi \leq 1/2$. For these values of χ the expression under the square root in (2.2) is negative and we thus get a unique solution (up to complex conjugation).

Theorem 2.1 *For $0 < \chi \leq 1/2$, let the coefficients γ_1, γ_2, γ_3, δ_1, δ_2, and δ_3 be defined by the above procedure. The exponential splitting schemes*

$$\Psi_h(\chi) = \mathrm{e}^{\gamma_3(\chi)hA}\mathrm{e}^{\delta_3(\chi)hB}\,\mathrm{e}^{\gamma_2(\chi)hA}\mathrm{e}^{\delta_2(\chi)hB}\,\mathrm{e}^{\gamma_1(\chi)hA}\mathrm{e}^{\delta_1(\chi)hB}$$

are then all of classical order $p = 3$. □

For some choices of χ the coefficients of $\Psi_h(\chi)$ have a quite simple form. A few examples are $\chi = 1/10$, where the coefficients are

$$\gamma_1 = \tfrac{13}{34} - \mathrm{i}\,\tfrac{\sqrt{3579}}{102}, \qquad \delta_1 = \tfrac{77}{260} - \mathrm{i}\,\tfrac{\sqrt{3579}}{780},$$

$$\gamma_2 = \tfrac{13}{34} + \mathrm{i}\,\tfrac{\sqrt{3579}}{102}, \qquad \delta_2 = \tfrac{1}{10},$$

$$\gamma_3 = \tfrac{4}{17}, \qquad \delta_3 = \tfrac{157}{260} + \mathrm{i}\,\tfrac{\sqrt{3579}}{780},$$

and the choice $\chi = 1/3$, which yields

$$\begin{aligned} \gamma_1 &= \tfrac{5}{12} + \mathrm{i}\,\tfrac{\sqrt{11}}{12}, & \delta_1 &= \tfrac{7}{30} + \mathrm{i}\,\tfrac{\sqrt{11}}{30}, \\ \gamma_2 &= \tfrac{5}{12} - \mathrm{i}\,\tfrac{\sqrt{11}}{12}, & \delta_2 &= \tfrac{1}{3}, \\ \gamma_3 &= \tfrac{1}{6}, & \delta_3 &= \tfrac{13}{30} - \mathrm{i}\,\tfrac{\sqrt{11}}{30}. \end{aligned}$$

A particular case is obtained for $\chi = 1/2$, where

$$\begin{aligned} \gamma_1 &= \tfrac{1}{2} + \mathrm{i}\,\tfrac{\sqrt{3}}{6}, & \delta_1 &= \tfrac{1}{4} + \mathrm{i}\,\tfrac{\sqrt{3}}{12}, \\ \gamma_2 &= \tfrac{1}{2} - \mathrm{i}\,\tfrac{\sqrt{3}}{6}, & \delta_2 &= \tfrac{1}{2}, \\ \gamma_3 &= 0, & \delta_3 &= \tfrac{1}{4} - \mathrm{i}\,\tfrac{\sqrt{3}}{12}, \end{aligned}$$

and the resulting scheme

$$\Psi_h(1/2) = \mathrm{e}^{\left(\frac{1}{4}-\mathrm{i}\frac{\sqrt{3}}{12}\right)hB}\,\mathrm{e}^{\left(\frac{1}{2}-\mathrm{i}\frac{\sqrt{3}}{6}\right)hA}\,\mathrm{e}^{\frac{1}{2}hB}\,\mathrm{e}^{\left(\frac{1}{2}+\mathrm{i}\frac{\sqrt{3}}{6}\right)hA}\,\mathrm{e}^{\left(\frac{1}{4}+\mathrm{i}\frac{\sqrt{3}}{12}\right)hB} \tag{2.3}$$

only requires, in average, the evaluation of four semigroup actions instead of the normal six, see also [16, eq. (23)] and [14].

Of course, the parameter χ can also be chosen complex. Even so, we will omit a further investigation since the derived family $\Psi_h(\chi)$ already includes schemes with coefficients possessing fairly small arguments.

2.2 Deriving schemes via compositions

A second approach is to identify the splitting scheme as a composition method, and then to use the following result; see [6, Theorem II.4.1 and Section II.5].

Lemma 2.1 *Let S_h be a one step method of classical order q. If*

$$\sigma_1 + \ldots + \sigma_m = 1 \qquad \textit{and} \qquad \sigma_1^{q+1} + \ldots + \sigma_m^{q+1} = 0, \tag{2.4}$$

then the composition method $S_{\sigma_m h} \ldots S_{\sigma_1 h}$ is at least of classical order $q+1$. □

Using this argument iteratively allows us to create splitting schemes with increasing classical orders. In the framework of analytic semigroups, however, this construction does not yield expedient methods of arbitrary orders by default. This is due to the fact that the arguments of the coefficients are added together in each composition step, which in the end may result in coefficients with non-positive real parts.

In conclusion, when using the strategy of composition to generate high order schemes for analytic semigroups, it is vital to find solutions of (2.4) with small arguments $\arg \sigma_\ell$ for $1 \le \ell \le m$.

Two term compositions

We will first consider compositions with $m=2$. As a concrete example, let us employ the Strang splitting

$$\Phi_h = \mathrm{e}^{\frac{1}{2}hB}\mathrm{e}^{hA}\mathrm{e}^{\frac{1}{2}hB},$$

which has classical order $p=2$, as our starting scheme S_h. We then proceed by introducing the following chain of two term compositions

$$\Phi_h(k,2) = \Phi_{\sigma_{k,2}h}(k-1,2)\,\Phi_{\sigma_{k,1}h}(k-1,2), \qquad k \geq 1,$$

where $\Phi_h(0,2) = \Phi_h$ and the coefficients $\sigma_{k,1}$ and $\sigma_{k,2}$ are solutions of (2.4) for $m=2$ and $q=k+1$. By eliminating one of the two variables, system (2.4) reduces to

$$\sigma^{q+1} + (1-\sigma)^{q+1} = 0 \qquad \text{or} \qquad \left(\frac{\sigma}{1-\sigma}\right)^{q+1} = -1. \tag{2.5}$$

By taking the logarithms, we easily derive that all solutions of (2.5) are given by

$$\sigma = \frac{1}{2} + \mathrm{i}\,\frac{\sin\left(\frac{2\ell+1}{q+1}\pi\right)}{2+2\cos\left(\frac{2\ell+1}{q+1}\pi\right)} \qquad \text{for} \begin{cases} -\frac{q}{2} \leq \ell \leq \frac{q}{2}-1 & \text{if } q \text{ is even,} \\ -\frac{q+1}{2} \leq \ell \leq \frac{q-1}{2} & \text{if } q \text{ is odd.} \end{cases}$$

Since the function

$$\frac{\sin x}{2+2\cos x}, \qquad -\pi < x < \pi,$$

is monotonically increasing, we get coefficients with the smallest angles for $\ell = 0$. We therefore obtain the following schemes with orders ranging from three to six.

Theorem 2.2 *Let $1 \leq k \leq 4$. Then the exponential splitting schemes $\Phi_h(k,2)$ with*

$$\sigma_{k,1} = \frac{1}{2} + \mathrm{i}\,\frac{\sin\bigl(\pi/(k+2)\bigr)}{2+2\cos\bigl(\pi/(k+2)\bigr)} \qquad \textit{and} \qquad \sigma_{k,2} = \overline{\sigma}_{k,1}$$

are of order $p = k+2$. □

Note that the above two term composition can not be made for $k \geq 5$ in the framework of analytic semigroups, as the splittings $\Phi_h(k,2)$ then have coefficients γ_j and/or δ_j with negative real parts. Further note that the third order splitting $\Psi(1/2)$, given in (2.3), coincides with $\Phi_h(1,2)$.

Symmetric three term compositions

In order to obtain methods of higher order, we have to increase the number m of terms in the composition. If the composition is symmetric, i.e., if $\sigma_{m-\ell+1} = \sigma_\ell$ for all ℓ, then the order of the resulting splitting scheme is even. Hence, if we make a symmetric composition with a splitting S_h of even order p, then the resulting scheme $S_{\sigma_m h} \dots S_{\sigma_1 h}$ obtains an order of $p+2$; see [6, Section II.3 and II.5]

As a first step, we construct symmetric three term compositions. Starting from the Strang splitting $\Phi_h(0,3) = \Phi_h$, we consider the following chain of compositions

$$\Phi_h(k,3) = \Phi_{\sigma_{k,1}h}(k-1,3)\,\Phi_{\sigma_{k,2}h}(k-1,3)\,\Phi_{\sigma_{k,1}h}(k-1,3), \qquad k \geq 1,$$

where the coefficients $\sigma_{k,1}$ and $\sigma_{k,2}$ are solutions of (2.4) for $m = 3$ and $q = 2k$. By eliminating $\sigma_{k,2}$ we obtain the polynomial

$$2\sigma^{q+1} + (1-2\sigma)^{q+1} = 0 \qquad \text{or} \qquad \left(\frac{\sigma}{1-2\sigma}\right)^{q+1} = -\frac{1}{2}. \tag{2.6}$$

By once again taking the logarithms, we have that the solutions of minimal argument are

$$\sigma_{k,1} = \frac{e^{\pi i/(2k+1)}}{2^{1/(2k+1)} + 2e^{\pi i/(2k+1)}} \qquad \text{and} \qquad \sigma_{k,2} = 1 - 2\sigma_{k,1}. \tag{2.7}$$

This results in the schemes below, with the orders ranging from four to eight.

Theorem 2.3 *Let* $1 \leq k \leq 3$. *Then the exponential splitting schemes* $\Phi_h(k,3)$ *with coefficients given by* (2.7) *are of order* $p = 2k+2$. □

For our purpose, the three term compositions are useless for $k \geq 4$, as the splittings $\Phi_h(k,3)$ then have coefficients with negative real parts.

Symmetric four term compositions

To gain even higher order schemes, we conclude by constructing symmetric four term compositions. Starting again from the Strang splitting $\Phi_h(0,4) = \Phi_h$, we consider the compositions

$$\Phi_h(k,4) = \Phi_{\sigma_{k,1}h}(k-1,4)\,\Phi_{\sigma_{k,2}h}(k-1,4)\,\Phi_{\sigma_{k,2}h}(k-1,4)\,\Phi_{\sigma_{k,1}h}(k-1,4), \quad k \geq 1,$$

where the coefficients $\sigma_{k,1}$ and $\sigma_{k,2}$ are solutions of (2.4) for $m = 4$ and $q = 2k$. By eliminating $\sigma_{k,2}$ we obtain the polynomial

$$\sigma^{q+1} + \left(\tfrac{1}{2} - \sigma\right)^{q+1} = 0 \qquad \text{or} \qquad \left(\frac{2\sigma}{1-2\sigma}\right)^{q+1} = -1. \tag{2.8}$$

The solutions with minimal arguments are then

$$\sigma_{k,1} = \frac{1}{4} + i\,\frac{\sin\big(\pi/(2k+1)\big)}{4 + 4\cos\big(\pi/(2k+1)\big)} \qquad \text{and} \qquad \sigma_{k,2} = \overline{\sigma}_{k,1}, \tag{2.9}$$

and we get the schemes below of orders ranging from four to fourteen.

Theorem 2.4 *Let* $1 \leq k \leq 6$. *Then the exponential splitting schemes* $\Phi_h(k,4)$ *with coefficients given by* (2.9) *are of order* $p = 2k+2$. □

For $k \geq 7$ the splittings $\Phi_h(k,4)$ have coefficients with negative real parts.

3 The framework of analytic semigroups and convergence results

We next present the framework of unbounded operators which enables us to prove that any exponential splitting method of classical order p, and with appropriate complex coefficients, will retain its order when applied to (1.1).

Henceforth, X will denote an arbitrary (complex) Banach space with norm $\|\cdot\|$, and the corresponding operator norm will also be referred to as $\|\cdot\|$. Furthermore, C will be a generic constant which assumes different values at different occurrences. In our analysis, an essential tool are compositions of the operators A and B that consist of exactly k factors. We will denote such terms generically by E_k. For instance,

$$E_3 \in \{AAA, AAB, ABA, BAA, ABB, BAB, BBA, BBB\}.$$

To enable our analysis, we will assume the following.

Assumption 3.1 The linear operators L, A and B, all generate analytic semigroups on X defined in the sector $\Sigma_\phi = \{z \in \mathbb{C} : |\arg z| < \phi\}$, for a given angle $\phi \in (0, \pi/2]$. Furthermore, the operators A and B satisfy the additional bounds

$$\|\mathrm{e}^{zA}\| \le \mathrm{e}^{\omega|z|} \quad \text{and} \quad \|\mathrm{e}^{zB}\| \le \mathrm{e}^{\omega|z|}$$

for some $\omega \ge 0$ and all $z \in \Sigma_\phi$.

Assumption 3.2 All expressions of the form $E_{p+1}u(t)$ are uniformly bounded on the interval $[0, T]$, for some $T > 0$.

See [5, Section II.4.a] or [13, Section 2.2.5] for an introduction to the theory of analytic semigroups. Under these assumptions it is possible to prove the following convergence results.

Theorem 3.1 *For the numerical solution of* (1.1)*, consider an exponential splitting method* (1.2) *of classical order p, with all its coefficients γ_j and δ_j in the sector $\Sigma_\phi \subset \mathbb{C}$. If Assumptions 3.1 and 3.2 are valid, then*

$$\big\|\big(S_h^n - \mathrm{e}^{nhL}\big)u_0\big\| \le Ch^p, \qquad 0 \le nh \le T,$$

where the constant C can be chosen uniformly on bounded time intervals and, in particular, independent of n and h.

Proof In our paper [7], we prove Theorem 3.1 for C_0 semigroups and exponential splitting schemes with real coefficients γ_j and δ_j; see [7, Theorem 2.3 and Section 4.4]. The proof is of an algebraic nature and when one has introduced the concept of analytic semigroups, as done in Assumption 3.1, it can be extended to the current setting of complex coefficients without changing any of the used arguments. □

As the discrete evolution operator S_h is complex valued, the above approach cannot be used directly to study problems in real Banach spaces X. A remedy would be to complexify X in the usual way to $X \oplus \mathrm{i}X$ with the norm

$$\|u + \mathrm{i}v\| = \max_{\alpha^2+\beta^2=1} \Big(\|\alpha u - \beta v\|^2 + \|\alpha v + \beta u\|^2\Big)^{1/2} \quad \text{for } u, v \in X,$$

see [15, Sect. 6.5]. For real initial data, the imaginary part of the numerical solution will stay $\mathscr{O}(h^p)$ on bounded time intervals. This follows at once from Theorem 3.1.

Another possibility, however, would be to restrict the numerical evolution after each time step to its real part. This is achieved by the projection operator

$$P : X \oplus \mathrm{i}X \to X : u + \mathrm{i}v \mapsto u.$$

As this projection satisfies $\|P\| = 1$, the modified flow

$$\widehat{S}_h = P S_h : X \to X \tag{3.1}$$

is power-bounded for $0 \le nh \le T$. This follows at once from Assumption 3.1. The global error at time $t = nh$ has the representation

$$\Big(\widehat{S}_h^n - \mathrm{e}^{nhL}\Big) u_0 = \sum_{j=0}^{n-1} \widehat{S}_h^{n-j-1} P \Big(S_h - \mathrm{e}^{hL}\Big) \mathrm{e}^{jhL} u_0,$$

and can be bounded in the same way as before. We thus get the following corollary.

Corollary 3.1 *For the numerical solution of* (1.1) *on a real Banach space, consider the splitting method* (3.1)*. If the assumptions of Theorem 3.1 are valid, then*

$$\big\| \big(\widehat{S}_h^n - \mathrm{e}^{nhL}\big) u_0 \big\| \le C h^p, \qquad 0 \le nh \le T,$$

where the constant C can be chosen uniformly on bounded time intervals and, in particular, independent of n and h. □

Note that the extension to splittings of more then two operators and variable step sizes presented in [7, Section 4] are also generalizable to the present context of complex coefficients.

As a direct consequence of Theorem 3.1, the splitting schemes derived in Section 2 retain their classical order when applied to problems satisfying Assumption 3.1 with a sufficiently large angle ϕ, i.e,

$$\phi > \varphi := \max\big(|\arg \gamma_1|, \ldots, |\arg \gamma_s|, |\arg \delta_1|, \ldots, |\arg \delta_s|\big).$$

Hence, when designing splitting schemes for evolution equations governed by semigroups one should try to minimize the method angle φ, as this gives rise to more widely applicable schemes. The orders and angles for the methods derived in Section 2 are presented in Tables 3.1 and 3.2.

Table 3.1 The method angles φ of the third order schemes presented in Section 2.1.

S_h	$\Psi_h(1/10)$	$\Psi_h(1/3)$	$\Psi_h(1/2)$
φ	56.90°	33.56°	30°

Table 3.2 The method angles φ and orders p for the composition schemes derived in Section 2.2.

S_h	$\Phi_h(0,2)$	$\Phi_h(1,2)$	$\Phi_h(2,2)$	$\Phi_h(3,2)$	$\Phi_h(4,2)$		
φ	0°	30°	52.50°	70.50°	85.50°		
p	2	3	4	5	6		
S_h	$\Phi_h(0,3)$	$\Phi_h(1,3)$	$\Phi_h(2,3)$	$\Phi_h(3,3)$			
φ	0°	37.47°	60.49°	77.11°			
p	2	4	6	8			
S_h	$\Phi_h(0,4)$	$\Phi_h(1,4)$	$\Phi_h(2,4)$	$\Phi_h(3,4)$	$\Phi_h(4,4)$	$\Phi_h(5,4)$	$\Phi_h(6,4)$
φ	0°	30°	48°	60.86°	70.86°	79.04°	85.96°
p	2	4	6	8	10	12	14

4 Dimension splitting of parabolic problems

In order to illustrate that Assumptions 3.1 and 3.2 are reasonable for parabolic equations and their dimension splittings, we give the following example:

Let Ω be a bounded domain in $\mathbb{R}^d$ with a sufficiently regular boundary $\partial\Omega$ and set $X = L^2(\Omega)$. Consider the dimension splitting of the elliptic operator $L = A+B$, where

$$Au = \sum_{i=1}^{s} D_i\,(a_i D_i u) \quad \text{and} \quad Bu = \sum_{j=s+1}^{d} D_j\,(a_j D_j u)\,,$$

the functions $a_i \in C^\infty(\overline{\Omega})$ are real and positive, and $D_i = \partial/\partial x_i$. Furthermore, we impose homogenous Dirichlet conditions on $\partial\Omega$.

To validate Assumption 3.1, we first restrict our attention to the operator A. The operator can be cast into the framework of analytic semigroups on X by introducing the sesquilinear form

$$b(u,v) = \sum_{i=1}^{s} \big(\sqrt{a_i} D_i u, \sqrt{a_i} D_i v\big),$$

where $(\cdot,\cdot)$ is the inner product on X. Next, define the Hilbert space V with inner product

$$(u,v)_V = \lambda\,(u,v) + b(u,v) \tag{4.1}$$

as the completion of $C_0^\infty(\Omega)$ with respect to the norm induced by (4.1). Here, λ is a given positive parameter. Note that this yields the following chain of imbeddings $V \hookrightarrow X \cong X' \hookrightarrow V'$, where X' denotes the dual space of X. With this construction it is possible to interpret A as an unbounded operator on X with domain

$$\mathscr{D}(A) = \{u \in V : \exists\, y \in X \text{ with } (y,v) = -b(u,v)\ \forall v \in V\}$$

and $Au = y$ for all $u \in \mathscr{D}(A)$. To establish the generating properties of A, we first observe that

$$(Au,u) = -b(u,u) \le 0 \qquad \text{for all } u \in \mathscr{D}(A). \tag{4.2}$$

Secondly, by the Riesz representation theorem, there exists a unique $u \in V$ for every $y \in X$ and $\lambda > 0$ such that

$$(u,v)_V = \lambda(u,v) + b(u,v) = (y,v) \qquad \text{for all } v \in V.$$

Hence, $u \in \mathscr{D}(A)$ and $(\lambda I - A)u = y$, which implies the range property $\mathscr{R}(\lambda I - A) = X$ for all $\lambda > 0$. In conclusion, the hypotheses of the Lumer–Phillips theorem are valid, and the operator A therefore generates a C_0 semigroup of contractions on X, i.e., e^{zA} is well defined for $z \in [0,\infty)$.

We will next extend the semigroup to a sector $\Sigma_\phi = \{z \in \mathbb{C} : |\arg z| < \phi\}$. To this end, note that the inequality (4.2) yields that the numerical range of A is contained in the interval $(-\infty, 0]$, and the range condition $\mathscr{R}(\lambda I - A) = X$ gives that the resolvent set of A, $\rho(A)$, contains the interval $(0,\infty)$. These properties together with [13, Theorem 1.3.9] implies the inclusion $\Sigma_\pi \subset \rho(A)$ and, for every $\varepsilon \in (0, \pi/2)$, the resolvent bound

$$\|(\lambda I - A)^{-1}\| \leq \frac{M_\varepsilon}{|\lambda|} \qquad \text{for all } \lambda \in \overline{\Sigma}_{\pi-\varepsilon} \setminus \{0\}.$$

This is the standard characterization of a generator of an analytic semigroup on X, defined in the sector $\Sigma_{\pi/2}$; see [5, Theorem II.4.6] or [13, Theorem 2.5.2]. The analytic semigroup e^{zA} is also contractive, i.e., $\|\mathrm{e}^{zA}\| \leq 1$ for all $z \in \Sigma_{\pi/2}$. This can be seen by integrating the inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\mathrm{e}^{tzA}u\|^2 = 2\,\mathrm{Re}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{tzA}u, \mathrm{e}^{tzA}u\Big) = 2\,\mathrm{Re}(z)\,\big(A\mathrm{e}^{tzA}u, \mathrm{e}^{tzA}u\big) \leq 0$$

from 0 to 1 with respect to t.

By merely changing the number of terms in the sesquilinear form $b(\cdot,\cdot)$ and renumbering the dimensions, we can do the same interpretation of the operators L and B, which validates Assumption 3.1 for $\phi = \pi/2$. One can also use similar techniques to show that Assumption 3.1 is valid for the periodic problem, i.e., Ω is a d-dimensional torus $\mathbb{T}^d$, or if one imposes Neumann boundary conditions. The same holds for the degenerate case as well, where the functions a_i vanish at the boundary $\partial\Omega$; see [8, Example 5.2] for more details.

Assumption 3.2 is valid whenever

$$\mathscr{D}(L^{p+1}) \subseteq \mathscr{D}(E_{p+1}), \tag{4.3}$$

as $\mathrm{e}^{tL} : \mathscr{D}(L^{p+1}) \to \mathscr{D}(L^{p+1})$ for all times $t \in [0,T]$. The periodic setting yields that $\mathscr{D}(L^{p+1}) = H^{2(p+1)}(\mathbb{T}^d)$, and inclusion (4.3) is then trivially verified for all $p \geq 1$. The same is true for the degenerate problem, but the situation becomes more delicate when boundary conditions are imposed. As a simple example, we consider the Dirichlet Laplacian $L = \Delta$ over the unit square $\Omega = (0,1)^2$. Here,

$$\mathscr{D}(L^{p+1}) = \{u \in H^{2(p+1)}(\Omega) \subset C^{2p}(\overline{\Omega}) :\ u = Lu = L^2u = \ldots L^p u = 0 \text{ on } \partial\Omega\},$$

and $Lu = (\partial_n^2 + \partial_t^2)u$ almost everywhere on $\partial\Omega$, where ∂_n and ∂_t denote the normal and tangential derivatives, respectively. If we start with $p = 1$, then

$$u \in \mathscr{D}(L^2) \quad \Rightarrow \quad \begin{cases} u = 0 & \Rightarrow \quad \partial_t^2 u = 0 \quad \text{a.e. on } \partial\Omega \\ Lu = 0 & \Rightarrow \quad \partial_n^2 u = Lu - \partial_t^2 u = 0 \quad \text{a.e. on } \partial\Omega \end{cases}$$
$$\Rightarrow \quad Au = Bu = 0 \quad \text{on } \partial\Omega.$$

Note that the almost everywhere part can be dropped as Au and Bu are both continuous on $\overline{\Omega}$. This implies the inclusion $\mathscr{D}(L^2) \subseteq \mathscr{D}(E_2)$. Continuing to $p = 2$, gives the additional condition

$$L^2 u = \big(\partial_n^4 + \partial_n^2\partial_t^2 + \partial_t^2\partial_n^2 + \partial_t^4\big)u = \big(\partial_n^4 + 2\partial_t^2\partial_n^2\big)u = 0 \quad \text{a.e. on } \partial\Omega,$$

but one knows nothing about, for example, $\partial_n^4 u$ alone which is needed to validate that $\mathscr{D}(L^3)$ is a subset of $\mathscr{D}(A^3) \cap \mathscr{D}(B^3)$. In conclusion, $\mathscr{D}(L^{p+1})$ can not be expected to be a subset of $\mathscr{D}(E_{p+1})$, for $p \geq 2$, when one considers boundary conditions in general.

5 Numerical experiments and implementation

As a final step, we will demonstrate the performance of the derived splitting schemes. To this end, consider the evolution equation (1.1) with

$$Lu = (A+B)u = D_1(aD_1u) + D_2(aD_2u),$$

in the four cases below.

[PER] The periodic case, where we set $\Omega = \mathbb{T}^2$, with coordinates $(x_1, x_2) \in [0,1)^2$,

$$a(x_1,x_2) = \sin(2\pi x_1)\sin(2\pi x_2) + 2 \quad \text{and} \quad u_0(x_1,x_2) = \sin(2\pi x_1)\sin(2\pi x_2).$$

[DEG] The degenerate case, i.e., a vanishes on $\partial\Omega$. Here, $\Omega = (0,1)^2$,

$$a(x_1,x_2) = 16x_1(1-x_1)x_2(1-x_2) \quad \text{and} \quad u_0(x_1,x_2) = \sin(3\pi x_1)\cos(3\pi x_2).$$

[DIR] The case of homogenous Dirichlet boundary conditions, for which $\Omega = (0,1)^2$,

$$a(x_1,x_2) = 16x_1(1-x_1)x_2(1-x_2) + 1 \quad \text{and} \quad u_0(x_1,x_2) = c\,\mathrm{e}^{-\frac{1}{x_1(1-x_1)} - \frac{1}{x_2(1-x_2)}},$$

where c is chosen such that $\|u_0\|_{L^\infty(\Omega)} = 1$.

[NEU] The case of homogenous Neumann boundary conditions, where we use the same Ω, a and u_0 as for DIR.

Table 5.1 The spatial steps k, grids Ω_k, and coefficients $a_{i,j}$ used in the numerical experiments.

Case	k	Ω_k	$a_{i,j}$
PER	$1/m$	$\{0,k,\ldots,(m-1)k\}^2$	$a\big((i-1)k,(j-1)k\big)$
DEG	$1/(m+1)$	$\{k,2k,\ldots,mk\}^2$	$a(ik,jk)$
DIR	$1/(m+1)$	$\{k,2k,\ldots,mk\}^2$	$a(ik,jk)$
NEU	$1/(m-1)$	$\{0,k,\ldots,(m-2)k,1\}^2$	$a\big((i-1)k,(j-1)k\big)$

Note that the initial values u_0 are all chosen as elements of the corresponding domain $\mathscr{D}(L^\infty)$. Next, we introduce the discrete operator $L_k = A_k + B_k$, given by the standard central difference scheme over the mesh Ω_k, where

$$(A_k u)_{i,j} = \frac{1}{k^2}\big(a_{i+1/2,j}(u_{i+1,j}-u_{i,j}) + a_{i-1/2,j}(u_{i-1,j}-u_{i,j})\big) \qquad \text{and}$$

$$(B_k u)_{i,j} = \frac{1}{k^2}\big(a_{i,j+1/2}(u_{i,j+1}-u_{i,j}) + a_{i,j-1/2}(u_{i,j-1}-u_{i,j})\big),$$

for $i,j=1,\ldots,m$. The spatial step k, the mesh Ω_k and the coefficient $a_{i,j}$ are presented in Table 5.1.

In all cases the ghost values ($u_{0,j}$, $u_{m+1,j}$, $u_{i,0}$, and $u_{i,m+1}$) are given via the boundary conditions, except in the case of DEG, where they are obtained via linear extrapolation; see [8, p. 11]. Furthermore, for PER and NEU the diffusion coefficients a are extended outside Ω in a periodic and symmetric fashion, respectively.

The operators A_k and B_k can be represented as $m^2 \times m^2$ matrices of the form

$$\begin{bmatrix} T_1 & & \\ & \ddots & \\ & & T_m \end{bmatrix},$$

where the $m \times m$ blocks T_i are tridiagonal (or almost tridiagonal in the case of PER). Hence, the computations of e^{zA_k} and e^{zB_k} are reduced to the computation of the terms e^{zT_i}. In the current implementation the matrices e^{zT_i} are simply computed by Matlab's *expm*-routine. If further efficiency is required, a possible alternative to the expm-routine would be to use Krylov type methods instead; see for example [9]. For our experiments we set $m = 100$ and the time stepping error at time $T = 0.1$ is then approximated, with respect to the discrete L^2-norm, by comparing with the solution obtained when using the full operator L_k and the 4-stage Radau IIA method with $T/h = 4096$.

The observed errors for the splittings $\Psi_h(1/3)$, Φ_h, $\Phi_h(1,2)$ and $\Phi_h(1,3)$, are presented in Figure 5.1, and the corresponding orders are given in Table 5.2. The simulations clearly display that the classical order p is obtained for all methods in the cases PER and DEG, hence, in full agrement with Theorem 3.1. As discussed in Section 4, Assumption 3.2 is in general not satisfied for the infinite dimensional operator L when one imposes boundary conditions, and the convergence order is then no longer guarantied. With this in mind, it comes as no surprise that we observe severe order reductions in the experiments with DIR and NEU. More precisely, schemes with

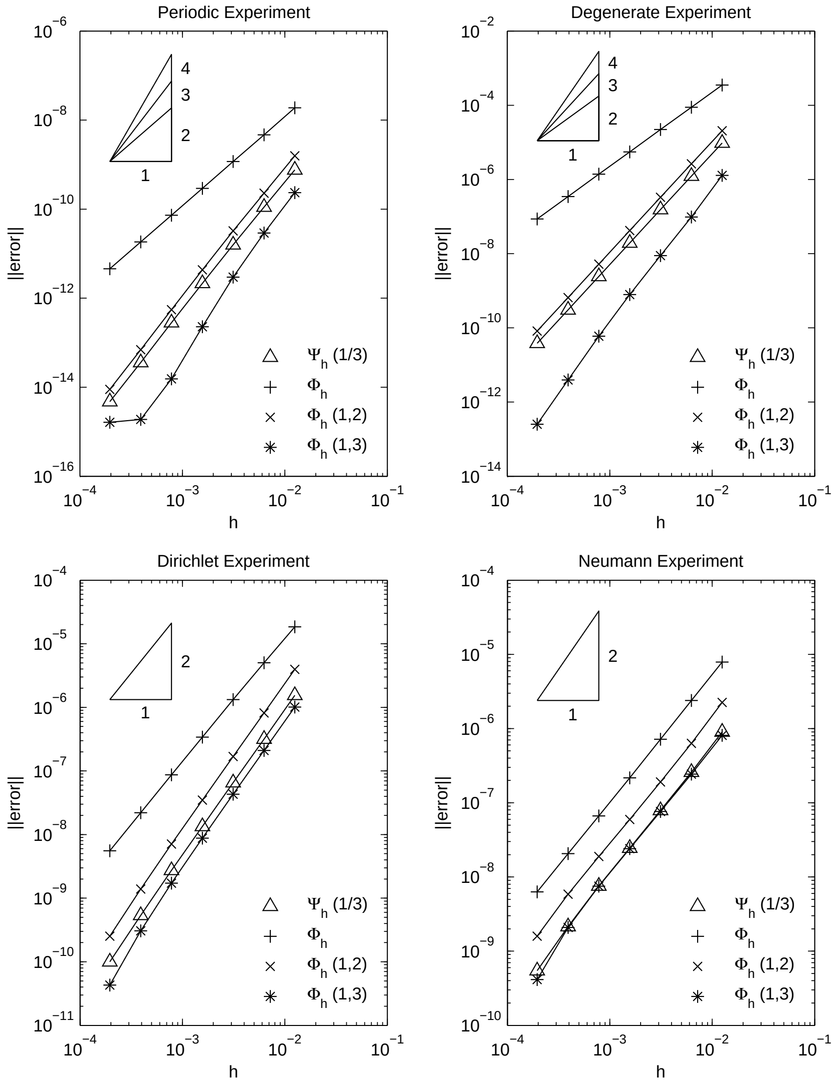

Fig. 5.1 The observed numerical errors with respect to the discrete L^2-norm, for a variety of splitting schemes. As seen from the graphs, the full convergence orders are obtained for the periodic and degenerate problems, whereas the order is reduced for all schemes with order $p \geq 3$ in the problems with Dirichlet and Neumann boundaries. Note that even though the full orders are not obtained in the Dirichlet and Neumann experiments, the high order schemes still yield significantly smaller errors when compared to the Strang splitting Φ_h.

Table 5.2 The observed numerical orders for a variety of splitting schemes.

Periodic Experiment

T/h	$\Psi_h(1/3)$	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
8				
16	2.77	2.02	2.78	3.02
32	2.82	2.00	2.82	3.29
64	2.87	2.00	2.91	3.70
128	2.94	2.00	2.97	3.90
256	2.97	2.00	2.99	3.03
512	2.93	2.00	2.95	0.21

Degenerate Experiment

T/h	$\Psi_h(1/3)$	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
8				
16	2.96	1.99	2.96	3.72
32	2.99	2.00	2.99	3.46
64	2.99	2.00	2.99	3.48
128	2.99	2.00	3.00	3.73
256	3.00	2.00	3.00	3.90
512	3.00	2.00	3.00	3.97

Dirichlet Experiment

T/h	$\Psi_h(1/3)$	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
8				
16	2.28	1.88	2.27	2.27
32	2.28	1.93	2.27	2.28
64	2.28	1.95	2.28	2.30
128	2.30	1.97	2.30	2.35
256	2.34	1.98	2.34	2.49
512	2.43	1.99	2.47	2.83

Neumann Experiment

T/h	$\Psi_h(1/3)$	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
8				
16	1.80	1.71	1.83	1.73
32	1.72	1.74	1.73	1.68
64	1.68	1.73	1.68	1.66
128	1.70	1.70	1.66	1.69
256	1.81	1.69	1.69	1.84
512	1.98	1.71	1.88	2.34

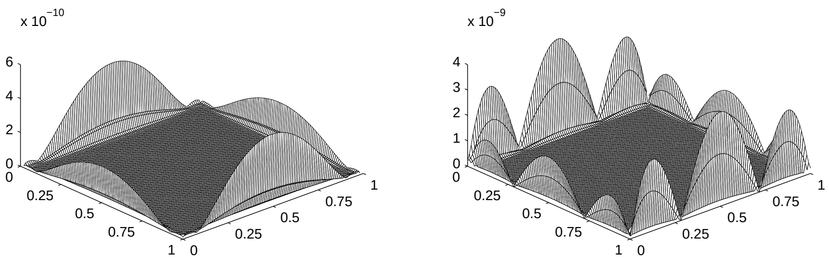

Fig. 5.2 The observed pointwise errors at time $T = 0.1$ for the splitting $\Phi_h(1,3)$, with $h = T/512$, when applied to the Dirichlet (left) and Neumann (right) problems. Note how the large errors are located along a thin strip around the boundary $\partial\Omega$.

$p \geq 3$ have an observed order of $p \approx 2.3$ in the case of DIR, and *all* consider schemes have an observed order of $p \approx 1.7$ for NEU.

As a final remark, we would like to point out that it may still be efficient to apply exponential splitting schemes of high order to parabolic problems with boundary conditions, as they often give rise to significantly smaller errors when compared to the Strang splitting Φ_h. Furthermore, the observed order reductions seem to originate only from the fact that the schemes yield large errors at, or very close to, the boundary; see Figure 5.2. Hence, the classical order is recovered sufficiently far inside the domain Ω, which can be rigorously proven by employing the techniques of [12].

However, we do not work out the details in this paper as the proof is rather lengthy and technical.

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