Non-existence of generalized splitting methods with positive coefficients of order higher than four

Winfried Auzinger

Technische Universität Wien, Institut für Analysis und Scientific Computing, Wiedner Hauptstrasse 8–10/E101, A-1040 Wien, Austria

Harald Hofstätter*

Universität Wien, Institut für Mathematik, Oskar-Morgenstern-Platz 1, A-1090 Wien, Austria

Othmar Koch

Universität Wien, Institut für Mathematik, Oskar-Morgenstern-Platz 1, A-1090 Wien, Austria

Abstract

We prove that generalized exponential splitting methods making explicit use of commutators of the vector fields are limited to order four when only real coefficients are admitted. This generalizes the restriction to order two for classical splitting methods with only positive coefficients.

Keywords: Non-reversible evolution equations, numerical time integration, generalized splitting methods, positive coefficients

2010 MSC: 65L05, 65L50

1. Introduction

1.1. Splitting methods

We consider evolution equations on $\mathbb{R}^d$ or $\mathbb{C}^d$ where the right-hand side is split into two components,

$$\partial_t y(t) = A(y(t)) + B(y(t)), \quad t \geq t_0, \quad y(t_0) = y_0. \quad (1)$$

In this introduction we only consider the linear case where $A, B$ are linear operators represented by real or complex matrices. For the numerical solution of (1)
we consider $s$-stage splitting methods, where one step $(t_n, y_n) \mapsto (t_{n+1}, y_{n+1})$ with step-size $\tau$ is given by
\[
y_{n+1} = S(\tau)y_n = e^{b_1 \tau B}e^{a_1 \tau A} \cdots e^{b_1 \tau B}e^{a_1 \tau A}y_n.
\] (2)
A splitting method has convergence order $p$ if it holds
\[
S(\tau)y_n = e^{\tau(A+B)}y_n + O(\tau^{p+1}).
\]

1.2. Positive coefficients
For certain applications only splitting schemes with non-negative coefficients are suitable. In particular this is the case if $A$ is a discretized sectorial operator associated with a parabolic equation, because in this case the flow of $A$ is non-reversible and does not tolerate negative time increments in the numerical approximation, whence $a_j$ is required to be non-negative. A splitting method of order $p = 2$ with all coefficients positive is given by Strang splitting
\[
S(\tau) = e^{\frac{\tau}{2}A}e^{\frac{\tau}{2}B}.
\]
It is known that $p = 2$ is the maximum order of a splitting method with all coefficients positive, a fact which is established by the following theorem.

**Theorem 1.** If $S$ is a splitting method (2) of order $p \geq 3$ with real coefficients, then at least one of the coefficients $a_j$ is strictly negative, and also at least one of the coefficients $b_j$ is strictly negative.

This theorem was first proved in [1], see also [2]. A weaker version stating that at least one of all coefficients $a_j$, $b_j$ combined is strictly negative, was proved earlier in [3).

1.3. Generalized splitting methods
In many applications the commutator $[B, [B, A]]$ and its exponential are readily computable, see [4]. This suggests to consider generalized splitting methods of the form
\[
y_{n+1} = S(\tau)y_n = e^{c_3 \tau^3[B,[B, A]]}e^{b_1 \tau B}e^{a_1 \tau A} \cdots e^{b_1 \tau B}e^{a_1 \tau A}y_n,
\] or
\[
y_{n+1} = S(\tau)y_n = e^{b_1 \tau B + c_3 \tau^3[B,[B, A]]}e^{a_1 \tau A} \cdots e^{b_1 \tau B + c_3 \tau^3[B,[B, A]]}e^{a_1 \tau A}y_n,
\]
which possibly allow orders higher than 2 while involving only positive coefficients. Indeed, the scheme
\[
S(\tau) = e^{\frac{\tau}{2}B}e^{\frac{\tau}{2}A}e^{\frac{\tau}{2}B - \frac{1}{2}c_3 \tau^3[B,[B, A]]}e^{\frac{\tau}{2}A}e^{\frac{\tau}{2}B}
\]
proposed in [2, 6] has order $p = 4$ and positive coefficients $a_j$ and $b_j$. However, as established by the following theorem, $p = 4$ is the maximum order of such a generalized splitting method with all coefficients $a_j$ positive. This holds even under the additional assumption $[B, [B, [B, A]]] = 0$, which in many applications is satisfied, see [4].
Theorem 2.

(i) If $S$ is a generalized splitting method of the form (3) or (4) of order $p \geq 5$ with real coefficients, then at least one of the coefficients $a_j$ is strictly negative.

(ii) If $S$ is a generalized splitting method (4) with real coefficients which is of order $p \geq 5$ if applied to an equation (1) where the operators $A, B$ satisfy $[B, [B, [B, A]]] = 0$, then at least one of the coefficients $a_j$ is strictly negative.

It is clear that part (i) follows immediately from part (ii), which immediately follows from the following theorem, which may be interesting in itself.

Theorem 3. If $S$ is a splitting method (2) with real coefficients which is of order $p \geq 5$ if applied to an equation (1) where the operators $A, B$ satisfy $[B, [B, [B, A]]] = 0$, then at least one of the coefficients $a_j$ is strictly negative.

A proof of Theorem 2 was proposed in [7]. In Section 2 we will give a new independent proof by showing that Theorem 3 (and thus also Theorem 2) is an easy consequence of a recent result proved by the authors in [8].

2. Proof of Theorem 3

The essential step leading to the main result of [8] is comprised by the following proposition.

Proposition 1. Let $u(t)$ be the exact solution of

$$\partial_t u(t) = H(t)u(t) = (H_0 + tH_1)u(t), \quad u(0) = u_0$$

with $H_0, H_1 \in \mathbb{C}^{d \times d}$ and

$$v(\tau) = e^{a_1 \tau H_0 + c_1 \tau^2 H_1} \cdots e^{a_s \tau H_0 + c_s \tau^2 H_1} u_0$$

with given coefficients $a_j, c_j \in \mathbb{R}$. If

$$v(\tau) - u(\tau) = O(\tau^6),$$

then at least one of the coefficients $a_j$ is strictly negative.\(^3\)

Here (6) can be interpreted as one step with step-size $\tau$ of a commutator-free exponential integrator applied to the special non-autonomous equation (5). To

---

\(^1\)By logical transposition: If an object (here a generalized splitting method with all coefficients $a_j$ nonnegative) does not exist under some restrictive assumptions, then it cannot exist under more general assumptions.

\(^2\)Note that we have changed some denotations: $H(t), H_0, H_1, s, a_j, c_j$ correspond respectively to the denotations $A(t), A_0, A_1, J, b_j, y_j$ of [8].

\(^3\)See Remark 2 below.
show that Theorem 3 follows from Proposition 1 we first use the standard reformulation
\[ y(t) = \begin{pmatrix} s(t) \\ u(t) \end{pmatrix}, \quad \partial_t y(t) = \begin{pmatrix} 0 \\ H(s(t))u(t) + (1) \end{pmatrix}, \quad y(0) = y_0 = \begin{pmatrix} 0 \\ u_0 \end{pmatrix} \] (7)
of the non-autonomous problem (5) as an autonomous problem by adding the component \( s(t) = t \). Here the operators \( A, B : \mathbb{R}^{d+1} \to \mathbb{R}^{d+1} \) are nonlinear, therefore a direct application of the splitting method (2) is not possible. However, by associating the flows \( E_A(t, y_0), E_B(t, y_0) \) of the subproblems \( \partial_t y(t) = A(y(t)), \partial_t y(t) = B(y(t)) \) with exponentials of Lie derivatives \( e^{tD_A}, e^{tD_B} \), which act on a smooth map \( F : \mathbb{R}^{d+1} \to \mathbb{R}^{d+1} \) as
\[
(e^{tD_A}F)(y) = F(E_A(t, y)) \quad \text{and} \quad (e^{tD_B}F)(y) = F(E_B(t, y)),
\]
and thus
\[
E_A(t, y_0) = (e^{tD_A}\text{Id})(y_0), \quad E_B(t, y_0) = (e^{tD_B}\text{Id})(y_0),
\]
each splitting method (2) of order \( p \) for linear problems (1) can be promoted to a splitting method
\[
y_{n+1} = S(\tau, y_n) = E_B(b_{s\tau}, \cdot) \circ E_A(a_{s\tau}, \cdot) \circ \ldots \circ E_B(b_{1\tau}, \cdot) \circ E_A(a_{1\tau}, y_n)
= (e^{a_{s\tau}D_A}e^{b_{1\tau}D_B} \ldots e^{a_{s\tau}D_A}e^{b_{s\tau}D_B}\text{Id})(y_n)
\] (8)
of the same order for nonlinear problems, see [9, Section III.5.1].

Remark 1. The convergence order of a (generalized) splitting method is determined by order conditions, which are polynomial equations in the coefficients of the method. Usually these conditions are derived in a purely formal way in the abstract algebra of formal power series in the non-commuting variables \( A, B \) and its embedded Lie algebra with Lie bracket defined by \([X, Y] = XY - YX\), see [10, 11]. By associating \( A, B \) with the matrices \( A, B \) in the linear case, and with the Lie derivatives \( D_A, D_B \) in the nonlinear case, it follows that (2) and (8) indeed have the same order [9].

For the special problem (7) the Lie derivatives are given by
\[
D_A = \sum_{i=1}^{d+1} A_i(y) \frac{\partial}{\partial y_i} = \sum_{i=1}^{d} [H(s)u]_i \frac{\partial}{\partial u_i} = \sum_{i=1}^{d} [(H_0 + sH_1)u]_i \frac{\partial}{\partial u_i}
\]
and
\[
D_B = \sum_{i=1}^{d+1} B_i(y) \frac{\partial}{\partial y_i} = \frac{\partial}{\partial s}
\]

\[\text{We adopt the notation from [9, Chapter III].}\]

4
A straightforward calculation leads to

\[ [D_B, D_A] = \sum_{i=1}^{d} [H'(s)u_i] \frac{\partial}{\partial u_i} = \sum_{i=1}^{d} [H_1u_i] \frac{\partial}{\partial u_i} \]

and

\[ [D_B, [D_B, D_A]] = \sum_{i=1}^{d} [H''(s)u_i] \frac{\partial}{\partial u_i} = 0, \]

which shows that the condition \([B, [B, A]] = 0\) of Theorem 3 promoted to the nonlinear case is satisfied. Repeated application of the formal identity

\[ e^X e^Y = e^Y + [X, Y] e^X \text{ for } [X, [X, Y]] = 0 \]

to (8) yields

\[ S(\tau, y_0) = (9) \]

with well-defined coefficients \(c_2, \ldots, c_s \in \mathbb{R}\). Here a single exponential acts as

\[ (e^{a_j \tau D_A + c_j \tau^2[D_B, D_A]} F \left( \begin{array}{c} s \\ u \end{array} \right) ) = F \left( e^{a_j \tau H(s) + c_j \tau^2 H'(s) u} \right) \]

and thus, substituting \(s = 0\),

\[ \left( e^{a_j \tau D_A + c_j \tau^2[D_B, D_A]} F \right) \left( \begin{array}{c} 0 \\ u \end{array} \right) = F \left( e^{a_j \tau H_0 + c_j \tau^2 H_1 u} \right) \]

It follows that for \(y_0 = \left( \begin{array}{c} 0 \\ u_0 \end{array} \right)\) the lower components of (9) can be written as

\[ e^{a_s \tau H_0 + c_s \tau^2 H_1} \ldots e^{a_2 \tau H_0 + c_2 \tau^2 H_1} e^{a_1 \tau H_0 u_0}, \]

which is of the form (10). From Proposition 1 it follows that if the splitting method (8) has order \(p \geq 5\) if applied to the special problem (7), or, a fortiori, if applied to nonlinear problems with \([B, [B, A]] = 0\) in general, then at least one of the coefficients \(a_j\) is strictly negative. We have thus proved the nonlinear version of Theorem 3. For similar formal reasons as in Remark 1, the linear version of Theorem 3 follows as well.

**Remark 2.** Strictly speaking, only a version of Proposition 7 with the weaker conclusion that at least one of the coefficients \(a_j\) is non-positive has been proved in (3). Since we may assume form the outset that \(a_j \neq 0\) for \(j = 2, \ldots, s\) in (2), it is clear that this weaker version already suffices for the proof of Theorem 3. Conversely, Proposition 7 follows from Theorem 3 as can be shown by a similar reasoning as before. Thus, the version of Proposition 7 given here follows from the weaker version proved in (3).

5 See footnote 5
Acknowledgements

This work was supported in part by the Vienna Science and Technology Fund (WWTF) [grant number MA14-002].

References

[1] D. Goldman, T. Kaper, nth-order operator splitting schemes and nonreversible systems, SIAM J. Numer. Anal. 33 (1) (1996) 349–367.

[2] S. Blanes, F. Casas, On the necessity of negative coefficients for operator splitting schemes of order higher than two, Appl. Numer. Math. 54 (1) (2005) 23–37.

[3] Q. Sheng, Solving linear partial differential equations by exponential splittings, IMA J. Numer. Anal. 9 (2) (1989) 199–212.

[4] I. Omelyan, I. Mryglod, R. Folk, Construction of high-order force-gradient algorithms for integration of motion in classical and quantum systems, Phys. Rev. E 66 (2002) 026701.

[5] M. Suzuki, New scheme of hybrid exponential product formulas with applications to quantum Monte–Carlo simulations, in: Computer Simulation Studies in Condensed-Matter Physics VIII, Springer-Verlag, Berlin Heidelberg, 1995, pp. 169–174.

[6] S. Chin, Symplectic integrators from composite operator factorizations, Phys. Lett. A 226 (1997) 344–348.

[7] S. Chin, Structure of positive decompositions of exponential operators, Phys. Rev. E 71 (2005) 016703.

[8] H. Hofstätter, O. Koch, Non-satisfiability of a positivity condition for commutator-free exponential integrators of order higher than four, Numer. Math. 141 (3) (2019) 681–691.

[9] E. Hairer, C. Lubich, G. Wanner, Geometric Numerical Integration, 2nd Edition, Springer-Verlag, Berlin–Heidelberg–New York, 2006.

[10] W. Auzinger, W. Herfort, Local error structures and order conditions in terms of Lie elements for exponential splitting schemes, Opuscula Math. 34 (2014) 243–255.

[11] H. Munthe–Kaas, B. Owren, Computations in a free Lie algebra, Phil. Trans. R. Soc. Lond. A 357 (1754) (1999) 957–981.