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Practical splitting methods for the adaptive integration of nonlinear evolution equations. Part I: Construction of optimized schemes and pairs of schemes

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Practical splitting methods for the adaptive integration of nonlinear evolution equations. Part I: Construction of optimized schemes and pairs of schemes

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Abstract We present a number of new contributions to the topic of constructing efficient higher-order splitting methods for the numerical integration of evolution equations. Particular schemes are constructed via setup and solution of polynomial systems for the splitting coefficients. To this end we use and modify a recent approach for generating these systems for a large class of splittings. In particular, various types of pairs of schemes intended for use in adaptive integrators are constructed.

Keywords Evolution equations · splitting methods · free Lie algebra · order conditions · local error · embedded methods

Mathematics Subject Classification (2000) 65J08, 65M15, 68R15, 68W30

1 Introduction

Operator splitting techniques for the efficient numerical integration of evolution equations

$$\partial_t u(t) = F(u(t)), \quad t \geq 0, \qquad u(0) \text{ given}, \tag{1.1}$$

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have become increasingly popular in recent years. Splitting the right-hand side $F(u)$ into two or more components in an appropriate way enables efficient and accurate approximations. In particular, a number of higher-order schemes with real or complex coefficients have been constructed and analyzed. Relevant contributions to this fields can, e.g., be found in [7, 8, 9, 11, 12, 14, 17, 18, 21].

We present some new contributions to this topic. At first we review of the approach from [2] for the automatic setup of order conditions represented by polynomial equations in the coefficients to be determined. Special cases involving symmetries or composition methods based on lower-order schemes can be treated as well. Splitting of the right-hand side of (1.1) into two or three components is considered.

The goal is to identify good schemes of a desired order p. 'Good' refers to a compromise between efficiency (minimizing effort) as well as accuracy (minimizing a measure for the the expected behavior of the local error). In particular, we focus on the constructions pairs of schemes of orders $(p, p+1)$, where a scheme of order p acts as a 'worker', while a related scheme of order $p+1$ plays the role of a 'controller' for the purpose of practical local error estimation. The idea of using pairs of embedded schemes (an idea related to Runge-Kutta pairs) is due to [16]. Via more flexible embeddings, optimized variants can be constructed. We also introduce alternative ways of constructing $(p, p+1)$-pairs.

The intended purpose is adaptive integration based on a reliable local error control. This topic has been studied in detail, in particular in the context of Schrödinger equations, in [3, 5, 4, 6]. In these papers, an alternative method for local error estimation has been constructed and analyzed. It is based on a computable high order approximation of an integral representation of the local error in terms of the defect of the numerical solution. While this approach is rather universal, using optimized pairs of schemes, if applicable, will be more efficient in many cases. For splitting into three components, efficient (pairs of) high-order schemes are significantly more difficult to find, and therefore one will resort the defect-based error estimator, see [6].

In Part II of this paper we will present a detailed study of adaptive integration, using both approaches for local error estimation, for different types of linear and nonlinear evolution equations.

Problem setting and notation. For an evolution equation (1.1) where the right-hand side is split into two components,

$$\partial_t u(t) = F(u(t)) = A(u(t)) + B(u(t)), \quad t \geq 0, \tag{1.2}$$

a single step of a multiplicative splitting scheme, starting from u and over a step of length h, is given by[1]

$$\mathscr{S}(h,u) = \mathscr{S}_s(h, \mathscr{S}_{s-1}(h, \ldots, \mathscr{S}_1(h,u))) \approx \phi_F(h,u)\,, \tag{1.3a}$$

with

$$\mathscr{S}_j(h,v) = \phi_B(b_j h, \phi_A(a_j h, v))\,, \tag{1.3b}$$

with appropriate coefficients a_j, b_j. More general schemes based on splitting into three operators are also considered, see Section 2.4, and a special case of additive splitting is also included, see Section 2.2.

The local error of a splitting step is denoted by

$$\mathscr{S}(h,u) - \phi_F(h,u) =: \mathscr{L}(h,u)\,, \tag{1.4}$$

[1] ϕ_F denotes the flow associated with the given evolution equation.

Contents. In Sections 2 and 3 we describe our approach for setting up the order conditions for different types of [pairs of] schemes. Some technical details concerning implementation of this setup procedure are given in Section 4. By solving the resulting polynomial systems we have constructed a number of new variants, and we have compiled a collection of practically relevant (old and new) schemes and pairs of schemes up to order $p = 6$. This collection can be found at

`http://www.asc.tuwien.ac.at/~winfried/splitting`

and is also to be expected to be extended in the future. We will refer to this throughout as reference [1] to avoid listing coefficients in the present paper for the sake of brevity. Remarks on the schemes collected in [1] are given in Section 5, and in Section 6 we present a numerical exampleM.

2 Order conditions

Many authors have contributed to the topic of finding good methods. For an overview on the topic see [7], [18]. Here we do not attempt to describe the relevant approaches and results in detail but mainly refer to work related to our present activity. For the relevant mathematical background we refer to [7, 14, 18].

Among many others, [8, 9, 11], and [12] are devoted to the construction of optimal higher-order methods with real or complex coefficients, either via composition or by solving a set of order conditions generated in different ways. Order conditions take the form of a polynomial system in the unknown coefficients or composition weights ω_μ, see Section 2.2. In the following we recapitulate and illustrate by examples how order conditions can be setup according to [2]. Later on we will also present optimized schemes and pairs of schemes obtained on the basis of this approach, where 'optimized' means that a measure for the local error is chosen as small as possible.

2.1 Setup of order conditions

There are different ways to generate a polynomial system representing the conditions on the splitting coefficients for a desired order p. An essential theoretical basis is the well-known Baker-Campbell-Hausdorff (BCH) formula, see for example [14].

The approach proposed in [2], which we follow here, also relies on the BCH formula, but order conditions are set up in a completely automatic way. Most of the schemes and pairs of schemes specified in [1] have been obtained on the basis of the algorithm from [2]. In the following we explain and illustrate this approach by means of examples. For the purpose of generating order conditions it is sufficient to consider the case of a linear operator split into two parts A and B. We denote

$$A_j = a_j A, \;\; B_j = b_j B, \quad j = 1 \ldots s.$$

For the linear case the local error (1.4) is of the form $\mathscr{L}(h)\,u$ with a linear operator $\mathscr{L}(h)$.

Consider the Taylor expansion of the local error[2] of a one-step method starting at u,

$$\mathscr{L}(h)\,u = \sum_{q=1}^{p} \tfrac{h^q}{q!}\,\tfrac{\mathrm{d}^q}{\mathrm{d}h^q}\,\mathscr{L}(0)\,u + \tfrac{h^{p+1}}{(p+1)!}\,\tfrac{\mathrm{d}^{p+1}}{\mathrm{d}h^{p+1}}\,\mathscr{L}(0)\,u + \mathscr{O}(h^{p+2}). \tag{2.1}$$

[2] By construction, $\mathscr{L}(0) = 0$ for any consistent scheme.

The method is of order p iff $\mathscr{L}(h) = \mathscr{O}(h^{p+1})$; thus the conditions for order p are given by

$$\tfrac{\mathrm{d}}{\mathrm{d}h}\mathscr{L}(0) = \ldots = \tfrac{\mathrm{d}^p}{\mathrm{d}h^p}\mathscr{L}(0) = 0. \tag{2.2}$$

For the case of a splitting method we have (with $\boldsymbol{k} = (k_1,\ldots,k_s) \in \mathbb{N}_0^s$)

$$\tfrac{\mathrm{d}^q}{\mathrm{d}h^q}\mathscr{L}(0) = \sum_{|\boldsymbol{k}|=q} \binom{q}{\boldsymbol{k}} \cdot \prod_{j=1}^{s} \sum_{l=0}^{k_j} \binom{k_j}{l} A_j^l B_j^{k_j-l} \;-\; (A+B)^q. \tag{2.3}$$

If the conditions (2.2) are satisfied up to a given order p, then the leading term of the local error is given by $\frac{h^{p+1}}{(p+1)!}\frac{\mathrm{d}^{p+1}}{\mathrm{d}h^{p+1}}\mathscr{L}(0)$. This leading error term is a linear combination of higher-order commutators of the operators A and B. As explained in [2], a non-redundant set of order conditions can be built in a recursive way by generating the symbolic expressions (2.3) for $q = 1,2,3,\ldots$ in terms of formally linear but non-commuting operators A,B, and identifying coefficients associated with power products of A- and B-factors which uniquely identifies a commutator out of an appropriate basis of Lie-elements. For this purpose we use the so-called Lyndon basis, also called Lyndon-Shirshov basis, of the free Lie algebra generated by A and B. The elements of this basis are represented by the (associative) Lyndon words over the alphabet $\{\mathtt{A},\mathtt{B}\}$, see Table 2.1.

q	ℓ_q	Lyndon words over the alphabet $\{\mathtt{A},\mathtt{B}\}$
1	2	A, B
2	1	AB
3	2	AAB, ABB
4	3	AAAB, AABB, ABBB
5	6	AAAAB, AAABB, AABAB, AABBB, ABABB, ABBBB
6	9	AAAAAB, AAAABB, AAABAB, AAABBB, AABABB, AABBAB, AABBBB, ABABBB, ABBBBB
7	18	...
8	30	...
9	56	...
10	99	...

Table 2.1 ℓ_q is the number of words of length q.

Let us first illustrate the procedure by means of a simple example.

Example 1 For $s = 2$ we have

$$\tfrac{\mathrm{d}}{\mathrm{d}h}\mathscr{L}(0) = \underline{(a_1+a_2-1)}A + \underline{(b_1+b_2-1)}B, \tag{2.4a}$$

$$\begin{aligned}\tfrac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0) = {} & ((a_1+a_2)^2-1)A^2 \\ & + \underline{(2a_2b_1-1)}AB + (2a_1b_1+2a_1b_2+2a_2b_2-1)BA \\ & + ((b_1+b_2)^2-1)B^2\,.\end{aligned} \tag{2.4b}$$

The basic consistency condition for order $p = 1$ is $\frac{\mathrm{d}}{\mathrm{d}h}\mathscr{L}(0) = 0$ which is equivalent to $a_1+a_2 = 1$ and $b_1+b_2 = 1$. Assuming these first-order conditions are satisfied, the second derivative $\frac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0)$, which now represents the leading error term, simplifies to the commutator expression

$$\tfrac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0) = \underline{(2a_2b_1-1)}\,[A,B]\,, \tag{2.5}$$

giving the additional condition $2\,a_2\,b_1 = 1$ for order $p = 2$. Assuming now that the conditions for $p = 2$ are satisfied, the third derivative $\frac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0)$, which will now represent the leading error term, is a linear combination of the commutators $[A,[A,B]]$ and $[[A,B],B]$, namely

$$\tfrac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0) = \underline{(3\,a_2^2\,b_1 - 1)}\,[A,[A,B]] + \underline{(3\,a_2\,b_1^2 - 1)}\,[[A,B],B]\,. \tag{2.6}$$

This computation can be automatized:

- Generate the representation (2.4a) of $\frac{\mathrm{d}}{\mathrm{d}h}\mathscr{L}(0)$ and extract coefficients of the Lyndon words `A` and `B`. This gives the first-order conditions $a_1 + a_2 = 1$ and $b_1 + b_2 = 1$.
- Generate the representation (2.4b) of $\frac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0)$. For a solution of the equations for order 1, the leading local error will have the form $\frac{h^2}{2}\,\frac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0)$ with $\frac{\mathrm{d}^2}{\mathrm{d}h^2}\mathscr{L}(0)$ from (2.5). The coefficient of $[A,B]$ in (2.5) is determined by extracting the coefficient of the Lyndon word `AB` in (2.4b). This gives the equation $2\,a_2\,b_1 = 1$ which, together with the first-order conditions, represents a set of conditions for order $p = 2$.
- Generate the representation of $\frac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0)$ (we do not display it here). For a solution of the equations for order 2, the leading local error will have the form $\frac{h^3}{6}\,\frac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0)$ with $\frac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0)$ from (2.6). The coefficients of $[A,[A,B]]$ and $[[A,B],B]$ in (2.6) are determined by extracting the coefficients of the Lyndon words `AAB` and `ABB` in the expression for $\frac{\mathrm{d}^3}{\mathrm{d}h^3}\mathscr{L}(0)$.

In the simple case considered here, there is a one-dimensional manifold of solutions for order $p = 2$, and for each solution $\{a_1,a_2,b_1,b_2\}$ the size of the coefficients in (2.6) is a quality measure.

If a scheme of order 3 is desired, the system of equations is augmented by the further equations $3\,a_2^2\,b_1 = 1$ and $3\,a_2\,b_1^2 = 1$. (For the case $s = 2$ displayed here, the resulting system of equations has no solution; we need $s \geq 3$.)

In general, for arbitrary s and p, this procedure is continued up to the desired order, by 'implicit recursive elimination' as described in [2], automatically producing a generically non-redundant set of order conditions for a desired order p. This process is based on a special bijection between (associative) Lyndon words and bracketed, non-associative versions of these words which, in our context, are identified with higher-order commutators representing basis elements for the free Lie algebra generated by A and B. The expanded version of such a commutator is a Lie polynomial in terms of the non-commutative variables A and B. The essential point is that *its leading monomial, with respect to (alphabetically increasing) lexicographical order, is precisely the monomial represented by the corresponding Lyndon word;* see [10].

In the following, the relation '`<`' refers to lexicographical order of words over the alphabet $\{\mathtt{A},\mathtt{B}\}$.

Example 2 Consider a scheme of order $p = 4$, i.e., assume that the conditions up to order $p = 4$ are satisfied. Then, $\frac{\mathrm{d}^5}{\mathrm{d}h^5}\mathscr{L}(0)$ is a linear combination of commutators, or non-associative words, listed below and represented by the six Lyndon words of length 5 (see Table 2.1),

$$\mathtt{AAAAB} < \mathtt{AAABB} < \mathtt{AABAB} < \mathtt{AABBB} < \mathtt{ABABB} < \mathtt{ABBBB}\,.$$

The commutators are bracketed, non-associative versions of these words,[3]

$$
\begin{aligned}
[A,[A,[A,[A,B]]]] &= \underline{A^4B} - 4A^3BA + 6A^2BA^2 - 4ABA^3 + BA^4\,,\\
[A,[A,[[A,B],B]]] &= \underline{A^3B^2} - 2\underline{\underline{A^2BAB}} + 4ABABA - AB^2A^2 - A^2B^2A - 2BABA^2 + B^2A^3\,,\\
[[A,[A,B]],[A,B]] &= \underline{A^2BAB} - A^2B^2A - 3ABA^2B + 4ABABA + 2BA^3B - 3BA^2BA\\
&\quad - AB^2A^2 + BABA^2\,,\\
[A,[[[A,B],B],B]] &= \underline{A^2B^3} - 3\underline{\underline{ABAB^2}} + 3AB^2AB - 2AB^3A + 3BAB^2A - 3B^2ABA + B^3A^2\,,\\
[[A,B],[[A,B],B]] &= \underline{ABAB^2} - 3AB^2AB + 2AB^3A - BA^2B^2 + 4BABAB - 3BAB^2A\\
&\quad - B^2A^2B + B^2ABA\,,\\
[[[[A,B],B],B],B] &= \underline{AB^4} - 4BAB^3 + 6B^2AB^2 - 4B^3AB + B^4A\,.
\end{aligned}
$$

As mentioned above, the leading (lowest) monomials in the expanded commutators, in the sense of lexicographical order, correspond to the Lyndon words. Note that some of these monomials also occur in lower commutators ('lower' again in the sense of lexicographical ordering). Let us now denote these six commutators by K_k, $k = 1\ldots6$. We a priori know that $\frac{\mathrm{d}^5}{\mathrm{d}h^5}\mathscr{L}(0)$ is of the form, with $\ell_5 = 6$,

$$\frac{\mathrm{d}^5}{\mathrm{d}h^5}\mathscr{L}(0) = \sum_{k=1}^{\ell_5} \kappa_k K_k$$

where the scalars κ_k are multivariate polynomials of degree 5 in the coefficients a_j, b_j of the underlying scheme of order $p = 4$. Therefore the additional conditions for order $p = 5$ are given by

$$\kappa_k = 0, \quad k = 1\ldots\ell_5\,. \tag{2.7a}$$

Extracting these coefficients κ_k from the expression (2.3) for $\frac{\mathrm{d}^5}{\mathrm{d}h^5}\mathscr{L}(0)$ is a combinatorial challenge, but we can do better: We simply extract the coefficients of the Lyndon monomials – let us denote them by λ_k – which is a standard operation in computer algebra. Now, instead of (2.7a) we require

$$\lambda_k = 0, \quad k = 1\ldots\ell_5\,. \tag{2.7b}$$

In our example, for $\boldsymbol{\kappa} = (\kappa_1,\ldots,\kappa_6)^T$ and $\boldsymbol{\lambda} = (\lambda_1,\ldots,\lambda_6)^T$ we have

$$\boldsymbol{\lambda} = M\boldsymbol{\kappa}, \quad \text{with} \quad M = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ -2 & & 1 & & & \\ & & & 1 & & \\ & & & -3 & 1 & \\ & & & & & 1 \end{pmatrix}, \tag{2.7c}$$

where the lower diagonal entries correspond to the additional occurrence of the λ_k in non-leading positions. Therefore the systems (2.7a) and (2.7b) are equivalent.

The situation displayed in this example occurs also in the general case. For any order p, the vectors $\boldsymbol{\kappa}$ and $\boldsymbol{\lambda}$ consisting of polynomials of degree $p+1$ satisfy $\boldsymbol{\lambda} = M\boldsymbol{\kappa}$ where M is a lower triangular matrix with unit diagonal. In particular, a Lyndon monomial λ_k never occurs in an expanded commutator K_j for $j > k$ because this would contradict the leading position [10] of the Lyndon monomial $\lambda_j > \lambda_k$ in K_j.

[3] The bracketing can be computed using the SageMath function `StandardBracketedLyndonWords`, see `www.sagemath.org`.

2.2 Special cases; symmetries

In the sequel,

$$\mathscr{S}^*(h,u) = \mathscr{S}^{-1}(-h,u)$$

denotes the adjoint scheme associated with $\mathscr{S}$.

The order conditions generated by the algorithm indicated in Section 2.1 are generically non-redundant. However, there exist special cases:

- *Symmetric* one-step schemes are characterized by the property

$$\mathscr{S}(-h,\mathscr{S}(h,u)) = u, \quad \text{i.e.,} \quad \mathscr{S}(h,u) = \mathscr{S}^*(h,u). \tag{2.8}$$

  For symmetric splitting schemes we have either $a_1 = 0$ or $b_s = 0$, and the remaining coefficient tupels (a_j) and (b_j) are both palindromic. Since symmetric schemes have an even order p (cf. [14, Chapter 3]), only odd-order conditions for an appropriately reduced number of free coefficients need to be imposed. The general algorithm described in Section 2.1 can easily be adapted to this case.
- The following type of schemes seems not to have been considered earlier in the literature:[4]
  Palindromic schemes, or 'reflected schemes' in the terminology of [2], are characterized by $b_j = a_{s+1-j}$, $j = 1 \ldots s$, i.e.,

$$\begin{aligned} &(a_1, b_1, a_2, b_2, \ldots, a_{s-1}, b_{s-1}, a_s, b_s) \\ = \; &(a_1, b_1, a_2, b_2, \ldots, b_2, \quad a_2, \quad b_1, a_1). \end{aligned}$$

  Assume a scheme of order p is given, and consider a splitting step of the form (1.3). Interchanging the roles of A and B, i.e., replacing (1.3) by

$$\check{\mathscr{S}}(h,u) = \check{\mathscr{S}}_s(h, \check{\mathscr{S}}_{s-1}(h, \ldots, \check{\mathscr{S}}_1(h,u))), \tag{2.9a}$$

  with

$$\check{\mathscr{S}}_j(h,v) = \phi_A(b_j h, \phi_B(a_j h, v)), \tag{2.9b}$$

  also results in a scheme of order p. If $\mathscr{S}$ is palindromic then

$$\mathscr{S}(-h,\check{\mathscr{S}}(h,u)) = u, \quad \text{i.e.,} \quad \check{\mathscr{S}}(h,u) = \mathscr{S}^*(h,u). \tag{2.10}$$

  Thus we infer from [14, Theorem II.3.2] that in the palindromic case the local errors $\mathscr{L}(h,u) = \mathscr{S}(h,u) - \phi_F(h,u)$ and $\check{\mathscr{L}}(h,u) = \check{\mathscr{S}}(h,u) - \phi_F(h,u)$ are related via

$$\mathscr{L}(h,u) = \quad C(u)\,h^{p+1} + \mathscr{O}(h^{p+2}), \tag{2.11a}$$

$$\check{\mathscr{L}}(h,u) = (-1)^p\, C(u)\,h^{p+1} + \mathscr{O}(h^{p+2}), \tag{2.11b}$$

  with $C(u) = \frac{1}{(p+1)!}\frac{\mathrm{d}^{p+1}}{\mathrm{d}h^{p+1}}\mathscr{L}(0,u)$. For an ansatz with palindromic coefficients, exchanging the role of A and B in the algorithm from Section 2.1 will lead to identical set of order conditions. Therefore the order conditions associated with 'Lyndon twins' are pairwise identical. Here, we call a pair of Lyndon words a twin if one of them is obtained by exchanging the role of A and B and reading it from right to left. See Table 2.1; for instance, the 6 words of odd length 5 consist of three twins; the 9 words of even length 6 consist of three twins, the selfie `AAABBB`, and two solitary words.
  Due to this redundancy, the number of order conditions is appropriately reduced.

[4] The Lie-Trotter scheme, with $s = p = 1$, $a_1 = b_1 = 1$, is a trivial special case.

– Higher order one-step schemes can be generated by m-fold *composition* of lower-order schemes with appropriately chosen sub-steps $h_\mu = \omega_\mu h$ satisfying $\omega_1 + \ldots + \omega_m = 1$ plus additional conditions guaranteeing that a certain order is obtained.[5]
A popular class of composition methods are symmetric Strang compositions. Schemes of this type of orders $4, 6$ and higher were first devised in [21]. Some of the composition coefficients have to be chosen negative, and the local error measures of these composition schemes are rather large. On the other hand, for higher orders, composition beats the generic lower limits on the number s of stages such that a given order p can be expected. For instance, the 7-fold 6-th order symmetric Strang composition [1, 'Y 8-6'] recombines into an 8-stage scheme, whereas the generic number of order conditions for a symmetric scheme of order $p = 6$ is 10, which would require $s = 10$ stages involving 11 free coefficients.

2.3 Complex coefficients

Our considerations are not restricted to schemes with real coefficients a_j, b_j. Complex schemes, with coefficients having positive real parts, are appropriate for the application of splitting methods to parabolic problems, since real schemes with positive coefficients do not exist for schemes of order $p \geq 3$, see [7]. For this class of methods, in particular based on complex compositions, we refer to [12] and [8].

2.4 Splitting into more than two operators

We also consider evolution equations where the right-hand side splits into three parts,

$$\partial_t u(t) = F(u(t)) = A(u(t)) + B(u(t)) + C(u(t)), \quad t \geq 0, \qquad u(0) \text{ given}, \tag{2.12}$$

and according multiplicative splitting schemes,

$$\mathscr{S}(h,u) = \mathscr{S}_s(h, \mathscr{S}_{s-1}(h, \ldots, \mathscr{S}_1(h,u))) \approx \phi_F(h,u), \tag{2.13a}$$

with

$$\mathscr{S}_j(h,v) = \phi_C(c_j h, \phi_B(b_j h, \phi_A(a_j h, v))). \tag{2.13b}$$

The methodology from [2] can be directly generalized to the case of splitting into more than two operators. For the practically relevant case of splitting into three operators A, B, C, as in (2.13), the representation (2.3) generalizes as follows, with $A_j = a_j A$, $b_j = b_j B$, $C_j = c_j C$, and $\boldsymbol{k} = (k_1, \ldots, k_s) \in \mathbb{N}_0^s$, $\boldsymbol{l} = (l_A, l_B, l_C) \in \mathbb{N}_0^3$:

$$\tfrac{\mathrm{d}^q}{\mathrm{d}h^q} \mathscr{L}(0) = \sum_{|\boldsymbol{k}|=q} \binom{q}{\boldsymbol{k}} \prod_{j=1}^{s} \sum_{|\boldsymbol{l}|=k_j} \binom{k_j}{\boldsymbol{l}} A_j^{l_A} B_j^{l_B} C_j^{l_C} \; - \; (A+B+C)^q. \tag{2.14}$$

On the basis of these identities, the algorithm from Section 2.1 generalizes in a straightforward way. The Lyndon basis representing independent commutators now corresponds to Lyndon words over the alphabet $\{\mathtt{A}, \mathtt{B}, \mathtt{C}\}$, see Table 2.2.

Concerning symmetries, similar considerations as in Section 2.2 apply.

[5] We note that the idea of composition is of a general nature and not restricted to the class of splitting methods.

q	ℓ_q	Lyndon words over the alphabet $\{\mathtt{A},\mathtt{B},\mathtt{C}\}$
1	3	A, B, C
2	3	AB, AC, BC
3	8	AAB, AAC, ABB, ABC, ACB, ACC, BBC, BCC
4	18	...
5	48	...
6	115	...
7	312	...
8	810	...

Table 2.2 ℓ_q is the number of words of length q.

For a general convergence theory of ABC-splitting for the linear case and some applications we refer to [6]. For example, splitting into three operators can be used to handle evolution equations where the right-hand side splits up into two non-autonomous parts. Introducing the independent variable t as an unknown variable satisfying $t' = 1$, such a problem can be formally considered as an autonomous system split into three parts. In this case, splitting means that the variable t is frozen over several subintervals comprising an integration step. Since the ODE $t' = 1$ is trivial, a large number of higher-order commutators vanishes in this case, and therefore the number of necessary order conditions is significantly reduced. This special situation will considered in detail later on.

3 Pairs of splitting schemes

For the purpose of efficient local error estimation as a basis for adaptive stepsize selection, using pairs of related schemes is a well-established idea. One of the schemes, of order p, acts as the worker, and the other, of order $p+1$, is the controller responsible for local error estimation.[6] Criteria for the selection of pairs of schemes are accuracy and computational efficiency.

Order conditions for pairs of schemes of the types listed below can be generated with minor modifications of the approach described in Section 2.

– *Embedded pairs.* In [16], pairs of splitting schemes of orders p and $p+1$ are specified. The idea is to select a controller $\bar{\mathscr{S}}$ of order $p+1$ and to construct a worker $\mathscr{S}$ of order p for which a maximal number of stages $\mathscr{S}_j$ coincides with those of the controller. Let a_j, b_j and $\bar{a}_j, \bar{b}_j$ denote the coefficients of the worker and controller, respectively. The approach adopted in [16] may be called static, finding $\mathscr{S}$ and $\bar{\mathscr{S}}$ such that $a_j = \bar{a}_j$ and $b_j = \bar{b}_j$ for as many $j = 1, 2, \ldots$ as possible. In this sense the schemes are related to each other but, in general, the total number of order conditions, and thus the total number of necessary evaluations, is the same as for an arbitrary unrelated $(p, p+1)$ pair.
Here we develop the idea of embedding further: Again we fix a 'good' controller of order $p+1$ and wish to adjoin to it a 'good' worker of order p. Since the number of stages $\bar{s}$ of $\bar{\mathscr{S}}$ will be higher than the number of stages s of $\mathscr{S}$, we can select an optimal embedded worker $\mathscr{S}$ from a set of candidates obtained by flexible embedding, where the number of coinciding coefficients is not a priori fixed.

Example 3 In [16], an embedded $(3,4)$-pair was constructed, where the controller is an optimized symmetric scheme of order $p = 4$ with $s = 7$ stages due to [9], with local error

[6] Of course, a scheme acting as a controller can also be used as an integrator in a normal way.

measure LEM=0.01 ('LEM' in the sense of (4.2b) below). The worker specified in [16] is a scheme of order $p = 3$ with $s = 6$ stages, where the coefficients a_1, a_2, a_3, a_4 and b_1, b_2, b_3 coincide with those of the controller. This amounts to 7 additional evaluations for the worker, and its local error measure is LEM=0.2.
For flexible embedding, in contrast, we consider all possible embedded workers, and we find that a scheme of order $p = 3$ with $s = 4$ stages is to be preferred, see [1, Emb 4/3 BM PRK/A], where a_1, a_2 and b_1 coincide with those of the controller. This amounts to 5 additional evaluations for the worker, and the controller has LEM=0.1.

– *Milne pairs.* In the context of multistep methods for ODEs, the so-called Milne device is a well-established technique for constructing pairs of schemes. In our context, one may aim for finding a pair $(\mathscr{S}, \tilde{\mathscr{S}})$ of schemes of equal order p such that their local errors $\mathscr{L}, \tilde{\mathscr{L}}$ are related according to

$$\mathscr{L}(h,u) = \ C(u)\,h^{p+1} + \mathscr{O}(h^{p+2}), \tag{3.1a}$$

$$\tilde{\mathscr{L}}(h,u) = \gamma C(u)\,h^{p+1} + \mathscr{O}(h^{p+2}), \tag{3.1b}$$

with $\gamma \neq 1$. Then, the additive scheme

$$\bar{\mathscr{S}}(h,u) = -\tfrac{\gamma}{1-\gamma}\,\mathscr{S}(h,u) + \tfrac{1}{1-\gamma}\,\tilde{\mathscr{S}}(h,u)$$

is a method of order $p+1$, and

$$\mathscr{S}(h,u) - \bar{\mathscr{S}}(h,u) = \tfrac{1}{1-\gamma}\left(\mathscr{S}(h,u) - \tilde{\mathscr{S}}(h,u)\right)$$

provides an asymptotically correct local error estimate for $\mathscr{S}(h,u)$.

– *Palindromic pairs.* Let $\mathscr{S}$ be a palindromic scheme of odd order p (see Section 2.2). Due to (2.11), the leading error terms of $\mathscr{S}$ and its adjoint $\mathscr{S}^* = \check{\mathscr{S}}$ are identical up to the factor -1. Therefore, the averaged additive scheme

$$\bar{\mathscr{S}}(h,u) = \tfrac{1}{2}\left(\mathscr{S}(h,u) + \check{\mathscr{S}}(h,u)\right) \tag{3.2}$$

is a method of order $p+1$,[7] and

$$\mathscr{S}(h,u) - \bar{\mathscr{S}}(h,u) = \tfrac{1}{2}\left(\mathscr{S}(h,u) - \check{\mathscr{S}}(h,u)\right)$$

provides an asymptotically correct local error estimate for $\mathscr{S}(h,u)$. In this case the additional effort for computing the local error estimate is identical with the effort for the worker $\mathscr{S}$ but not higher as is the case for embedded pairs.

For detailed comments on a number of new pairs listed in [1], see Section 5.

4 Implementation aspects: constructing schemes and minimizing local error terms

Our approach for setting up order conditions described in Section 2.1 has been implemented in[8] Maple 18. We use the `Physics` package for the manipulation of noncommuting symbols, and tables of Lyndon words generated using an algorithm devised in [13]. Since the number of terms in (2.3) resp. (2.14) rapidly increases with q we have implemented a parallel version

[7] For the simplest case of the Lie-Trotter scheme this was has already been observed in [19].

[8] Maple is a product of Maplesoft™.

relying on Maple's `Grid` package. In particular, the job of generating all the terms in the long sums (2.3) and (2.14) can be (equi-)distributed over several parallel threads.

The resulting set of order conditions is a multivariate polynomial system which, for higher orders, requires numerical solution techniques. Once a scheme of order p has been found, its leading local error term is of the form (see Section 2)

$$\tfrac{h^{p+1}}{(p+1)!}\,\tfrac{\mathrm{d}^{p+1}}{\mathrm{d}h^{p+1}}\mathscr{L}(0) = \sum_{k=1}^{\ell_{p+1}} \kappa_{p+1,k}\,K_{p+1,k}, \tag{4.1}$$

with ℓ_{p+1} commutators $K_{p+1,k}$ associated with Lyndon words of length $p+1$. To compare schemes of equal order p one may consider

$$\Big(\sum_{k=1}^{\ell_{p+1}} |\kappa_{p+1,k}|^2\Big)^{1/2} \tag{4.2a}$$

as a plausible measure for the accuracy of a scheme. However, we use the quantity

$$\mathrm{LEM} := \Big(\sum_{k=1}^{\ell_{p+1}} |\lambda_{p+1,k}|^2\Big)^{1/2}, \tag{4.2b}$$

instead. Using (4.2b) has the advantage that the coefficients $\lambda_k = \lambda_{p+1,k}$ are exactly those which are generated in course of the setup of the conditions for order $p+1$, see Section 2.1, while the coefficients from (4.2a) are more difficult to compute (cf. the discussion in Section 2.1). Since different particular solutions to the order conditions typically result in leading local error terms varying over several orders of magnitudes, we consider (4.2b) equally reasonable as (4.2a).

For finding and evaluating solutions and pairs of solutions we follow two different strategies.

- For the case where the number of equations equals the number of free coefficients we expect a set of isolated solutions. In this case we use the `fsolve` function in Maple combined with a Monte-Carlo strategy for generating different initial intervals. Higher precision is used to generate solutions with double precision accuracy. For each detected solution the LEM (4.2b) is computed.
- Especially for the case where the number of equations is smaller than the number of free coefficients, the problem is to be considered as a constrained minimization problem: Minimize the LEM representing the objective function, with the order conditions imposed as nonlinear equality constraints. To this end we employ state-of-the-art techniques which have also been applied for the construction of special classes Runge-Kutta methods, see for instance [15]. In particular we have used the MATLAB[9] optimizer `fmincon`. Again a large number of initial guesses are generated randomly, since this optimization problem is nonconvex in general. The results cannot be guaranteed globally optimal, but results from an exhaustive search usually suggest that this is indeed the case.

  A post-processing, i.e., refining the solutions to full double precision, is again performed in Maple using higher precision `sfloat` arithmetic.

We have also re-checked a number of known methods, refined their coefficients to full double precision, and computed their LEMs.

[9] MATLAB is a trademark of The Math Works, Inc.

5 Schemes from the collection [1]

This collection is not intended to be exhaustive. We present a number of relevant old and new schemes, in particular pairs of schemes, up to order $p = 6$, with their essential properties. Some methods are included mainly for the sake of completeness or their historical significance.

In the following we comment on some of these methods; for complete information, consult [1]. 'Best' or 'optimal' means that it has minimal LEM (4.2b) among a certain class of methods with comparable effort for a given order p. In some simple cases such optimality properties can be established theoretically; for higher orders we have resorted to more or less exhaustive numerical search.

Methods whose label contains the letter `'A'` are new, or taken again into consideration in the context of constructing pairs, or their LEM has been computed for the first time.[10] The list also includes some pairs of embedded schemes (`'Emb ...'`), pairs of Milne type (`'Milne ...'`), and palindromic pairs (`'PP ...'`), see Section 3.

5.1 Splitting into two operators ('AB schemes')

Real coefficients.

- The best schemes up to order $p = 5$ we have found are palindromic:
  - `'best 2-stage 2nd order'` ($s = p = 2$).
  - `'Emb 3/2 AKS'` (palindromic controller with $s = p = 3$).
  - `'Emb 4/3 AKS p'` (palindromic controller with $s = 5$, $p = 4$).
    In particular, this scheme has essentially the same LEM as the fourth order scheme from [9] which has been used in [16], but it has only only 5 stages instead of 7.
  - `'Emb 5/4 A'` (palindromic controller with $s = 8$, $p = 5$), see also `'PP 5/6 A'`.
- `'Emb 5/4 AK (ii)'` is an optimized embedded pair. The controller is a new scheme with $s = 7$, $p = 5$, and the worker of order $p = 4$ is chosen out of several dozens of candidates of order 4 which share the same computational effort but have LEMs varying over several orders of magnitudes.
- Palindromic pairs: `'PP 3/4 A'`, `'PP 5/6 A'`.

Complex coefficients (with positive real parts).

- Since for order $p = 3$ we need 5 conditions, the question is whether there exists a third-order scheme with $s = 3$ and 5 evaluations. It turns out that the only scheme of this type, `'A 3-3 c'`, has complex coefficients.
- `'A 4-4 c'` ($s = 4$, $p = 4$) is the best complex symmetric Strang composition method of order 4; see also [11] and [12].
- `'Emb 3/2 A c'` and `'Emb 4/3 A c'` are embedded pairs with palindromic controller and optimized worker. We note that the controller in `'Emb 4/3 A c'` ($s = 5$, $p = 4$) has a significantly smaller LEM than `'A 4-4 c'` (factor ≈ 20).
- `'C 8-6 c'` ($s = 8$, $p = 6$) is the best symmetric complex Strang composition method of order 6; see also [11] and [12].
- Palindromic pairs: `'PP 3/4 A c'`, `'PP 5/6 A c'`.

[10] Of course, 'new' may not be considered as a rigorous statement in each case since the literature on the subject is rather large by now.

5.2 Splitting into three operators ('ABC schemes')

Due to the rapidly increasing number of generic order conditions, finding general higher order schemes would be a very challenging task. For $p = 6$, for instance, the generic number of order conditions is 196 for the general case and 59 for the symmetric case. For $p = 6$ we therefore only consider real or complex Strang compositions, which are easier to construct. Generating the expression for the leading error term $\frac{\mathrm{d}^7}{\mathrm{d}h^7}\mathscr{L}(0)$ for the purpose of computing the LEM for $p = 6$, involving 312 coefficients (see Table 2.2), is computationally expensive.

Real coefficients.

- `'AK 5-2'` ($s = 5$, $p = 2$, 9 evaluations) appears to be a possible rival of the Strang scheme ($s = 3$, $p = 2$, 5 evaluations), with a LEM which is smaller by a factor ≈ 7.
- `'PP 3/4 A 3'` is a palindromic pair based on the best palindromic scheme found for $s = 6$, $p = 3$.
- `'Y 7-4'` ($s = 7, p = 4$, 13 evaluations) is the best symmetric Strang composition of order $p = 4$. It is the analog of the AB composition `'Y 4-4'`, with the same composition weights.
- `'AK 11-4'` ($s = 11$, $p = 4$, 21 evaluations) has been found on the basis of 11 conditions for a symmetric ABC scheme of order 4. Its LEM is smaller by a factor ≈ 13 compared to `'Y 7-4'`.
- `'AY 15-6'` ($s = 15, p = 6$) is the best symmetric Strang composition of order $p = 6$. It is the analog of the AB composition `'Y 8-6'`, with the same composition weights.

Complex coefficients (with positive real parts).

- `'AK 7-4 c'` ($s = 7, p = 4$) is the best symmetric Strang composition of order $p = 4$. It is the analog of the AB composition `'A 4-4-c'`, with the same composition weights.
- `'AK 15-6 c'` ($s = 15, p = 6$) is the best symmetric Strang composition of order $p = 6$. It is the analog of the AB composition `'C 8-6-c'`, with the same composition weights.

6 Numerical example

For a numerical illustration, in particular concerning the expected performance of palindromic schemes, we consider the system of coupled nonlinear Schrödinger equations (see [20])

$$\begin{aligned} \mathrm{i}\Big(\frac{\partial \psi_1}{\partial t} + \delta\frac{\partial \psi_1}{\partial x}\Big) + \frac{1}{2}\frac{\partial^2 \psi_1}{\partial x^2} + \big(|\psi_1|^2 + e\,|\psi_2|^2\big)\psi_1 = 0, \\ \mathrm{i}\Big(\frac{\partial \psi_2}{\partial t} - \delta\frac{\partial \psi_2}{\partial x}\Big) + \frac{1}{2}\frac{\partial^2 \psi_2}{\partial x^2} + \big(e\,|\psi_1|^2 + |\psi_2|^2\big)\psi_2 = 0, \end{aligned} \tag{6.1}$$

with exact solution (a pair of solitons)

$$\psi_1(x,t) = \frac{\sqrt{2\beta}}{1+e}\,\mathrm{sech}\big(\sqrt{2\beta}\,(x-vt)\big)\,\mathrm{e}^{\mathrm{i}\left((v-\delta)x+(\beta-(v^2-\delta^2)/2)t\right)},$$

$$\psi_2(x,t) = \frac{\sqrt{2\beta}}{1+e}\,\mathrm{sech}\big(\sqrt{2\beta}\,(x-vt)\big)\,\mathrm{e}^{\mathrm{i}\left((v+\delta)x+(\beta-(v^2-\delta^2)/2)t\right)},$$

which is exponentially decreasing with $|x|$. We start at $t = 0$, the parameters are chosen as $\delta = 0.5$, $\beta = 1.0$, $v = 1.1$, and $e = 0.8$.

We impose periodic boundary conditions on the interval $x_{min}, x_{max} = [-50, 70]$ using an equidistant grid of size 2.048. For splitting we choose the time step h and separately integrate

- the kinetic part ('A') involving the derivatives w.r.t. x, using a Fourier spectral discretization,
- and the nonlinear 'ODE part' ('B'), which can be exactly propagated: At each grid point x, the respective solution $(\psi_{1,B}, \psi_{2,B}) = (\psi_{1,B}(x,t), \psi_{2,B}(x,t))$ of the ODE system

$$\mathrm{i}\,\frac{\mathrm{d}\psi_{1,B}}{\mathrm{d}t} + \left(|\psi_{1,B}|^2 + e\,|\psi_{2,B}|^2\right)\psi_{1,B} = 0,$$
$$\mathrm{i}\,\frac{\mathrm{d}\psi_{2,B}}{\mathrm{d}t} + \left(e\,|\psi_{1,B}|^2 + |\psi_{2,B}|^2\right)\psi_{2,B} = 0,$$

starting at t_0 is given by

$$\psi_{1,B}(x,t) = \mathrm{e}^{\mathrm{i}\Delta t\,(|\psi_{1,B}(x,t_0)|^2 + e\,|\psi_{2,B}(x,t_0)|^2)}\,\psi_{1,B}(x,t_0),$$
$$\psi_{2,B}(x,t) = \mathrm{e}^{\mathrm{i}\Delta t\,(e\,|\psi_{1,B}(x,t_0)|^2 + |\psi_{2,B}(x,t_0)|^2)}\,\psi_{2,B}(x,t_0),$$

with $\Delta t = t - t_0$.

All computations were performed in standard double precision arithmetic. In Tables 6.1 and 6.2, 'err' refers to a canonically scaled discrete L_2, norm, and 'ord' refers to the order observed.

	scheme (i)		scheme ((i)+(ii))/2	
h	err_{local}	ord_{local}	err_{local}	ord_{local}
0.100 E+00	0.524 E−03		0.120 E−03	
0.500 E−01	0.374 E−04	3.74	0.467 E−05	4.69
0.250 E−01	0.246 E−05	3.93	0.150 E−06	4.96
0.125 E−01	0.156 E−06	3.98	0.468 E−08	5.01
0.625 E−02	0.982 E−08	3.99	0.146 E−09	5.00
0.313 E−02	0.614 E−09	4.00	0.455 E−11	5.00
0.156 E−02	0.384 E−10	4.00	0.142 E−12	5.00
0.781 E−03	0.240 E−11	4.00	0.456 E−14	4.96

scheme (i)	
err_{global}	ord_{global}
0.165 E−02	
0.106 E−03	3.96
0.912 E−05	3.54
0.100 E−05	3.18
0.123 E−06	3.03
0.154 E−07	2.99
0.194 E−08	2.99
0.244 E−09	2.99

Table 6.1 Error tables for the palindromic pair `'PP 3/4 A'` applied to problem (6.1). **Left:** Local error (first step) for scheme (i) starting with 'A' of order 3, and for the averaged scheme (see (3.2)) of order 4. **Right:** Global error for scheme (i) at $t_{end} = 5.0$.

	scheme (i)		scheme ((i)+(ii))/2	
h	err_{local}	ord_{local}	err_{local}	ord_{local}
0.100 E+00	0.322 E−04		0.318 E−04	
0.500 E−01	0.590 E−06	5.77	0.578 E−06	5.78
0.250 E−01	0.723 E−08	6.35	0.625 E−08	6.53
0.125 E−01	0.903 E−10	6.32	0.534 E−10	6.87
0.625 E−02	0.129 E−11	6.13	0.427 E−12	6.97

scheme (i)	
err_{global}	ord_{global}
0.166 E−02	
0.189 E−05	6.45
0.229 E−07	6.37
0.408 E−09	5.81
0.719 E−11	5.83

Table 6.2 Error tables for the palindromic pair `'PP 5/6 A'` applied to problem (6.1). **Left:** Local error (first step) for scheme (i) starting with 'A' of order 5, and for the averaged scheme (see (3.2)) of order 6. **Right:** Global error for scheme (i) at $t_{end} = 5.0$.

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