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Abstract

We demonstrate how a multiplicative splitting method of order P can be used to construct an additive splitting method of order $P+3$. The weight coefficients of the additive method depend only on P, which must be an odd number. Specifically we discuss a fourth-order additive method, which is yielded by the Lie-Trotter splitting. We provide error estimates, stability analysis, and numerical examples with the special discussion of the parallelization properties and applications to nonlinear optics.

1 Introduction

Splitting methods (SMs) are widely used for the solution of various linear and nonlinear evolution problems of mathematical physics in one or several spatial dimensions [26, 25, 22, 20]. Consider an abstract initial value problem within a sufficiently short evolution step τ

$$\frac{d}{dt}u(t) = Hu(t), \quad u(0) = u_0, \quad t \in [0,\tau], \quad H = \sum_{m=1}^{M} H_m, \tag{1}$$

where $u(t)$ belongs to a finite or infinite dimensional Banach space and a possibly unbounded evolution operator H generates a semigroup e^{tH} with $u(t) = e^{tH}u_0$. The evolution operator is split in M "reasonably simple" components H_m, such that the reduced equations $du/dt = H_m u$ can easily be addressed and generate individual semigroups.

An intermediate approximation $w_1(\tau)$ of $u(\tau)$ is yielded by solution of the sub-problem

$$\frac{d}{dt}w_1(t) = H_1 w_1(t), \quad w_1(0) = u_0, \quad t \in [0,\tau]. \tag{2}$$

The next intermediate approximation $w_2(\tau)$ is yielded by

$$\frac{d}{dt}w_2(t) = H_2 w_2(t), \quad w_2(0) = w_1(\tau), \quad t \in [0,\tau], \tag{3}$$

and so on, till $w_M(\tau)$ is calculated from $w_M(0) = w_{M-1}(\tau)$ by employing $e^{\tau H_M}$. The value $w_M(\tau)$ is then used as a final numerical approximation of the exact solution $u(\tau)$, such that

$$u_0 \xrightarrow{e^{\tau H_1}} w_1(\tau) \xrightarrow{e^{\tau H_2}} w_2(\tau) \xrightarrow{e^{\tau H_3}} \cdots \xrightarrow{e^{\tau H_{M-1}}} w_{M-1}(\tau) \xrightarrow{e^{\tau H_M}} w_M(\tau), \tag{4}$$

$$u(\tau) = e^{\tau H}u_0 \approx e^{\tau H_M} \cdots e^{\tau H_2} e^{\tau H_1} u_0. \tag{5}$$

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If an applied evolution problem is solved numerically, the interval $[0, \tau]$ in Eq. (1) mimics one time step. The sequence of the exponential operators $e^{\tau H_m}$, $1 \le m \le M$, at the right-hand-side of Eq. (5) defines the SM.

Generally, the components H_m do not commute, they can be applied in different order producing up to $M!$ SMs for a given splitting of H. The local error of a given SM can be characterised by the operator

$$\ell(e^{\tau H_M} \cdots e^{\tau H_2} e^{\tau H_1}) = e^{\tau H_M} \cdots e^{\tau H_2} e^{\tau H_1} - e^{\tau H} = O(\tau^2),$$

where the error estimate follows from the Taylor expansion. Any SM produces at least a first-order integrator when the basic Eq. (1) is solved on a fixed time domain by applying small τ-steps. One can do better than that and a SM is said to be of order p if its local error is $O(\tau^{p+1})$.

We denote SMs by capital calligraphic letters and indicate the time step by the index τ. The local error of a SM $\mathcal{M}_\tau$ of order p is denoted by $\ell(\mathcal{M}_\tau) = O(\tau^{p+1})$, in which case we write $\deg(\mathcal{M}_\tau) = p$. In what follows, the operator H in Eq. (1) will be divided in just two parts, $H = A + B$, and yet many different choices of the components H_m are possible. Some classical examples are as follows.

The simplest first-order Lie-Trotter SM, which is denoted by $\mathcal{L}_\tau$, reads [35]

$$\mathcal{L}_\tau = e^{\tau B} e^{\tau A} \quad \text{with} \quad \ell(\mathcal{L}_\tau) = e^{\tau B} e^{\tau A} - e^{\tau (A+B)} = O(\tau^2).$$

A second-order Strang SM, which is denoted by $\mathcal{S}_\tau$, reads [31]

$$\mathcal{S}_\tau = e^{\frac{1}{2}\tau A} e^{\tau B} e^{\frac{1}{2}\tau A} \quad \text{with} \quad \ell(\mathcal{S}_\tau) = O(\tau^3).$$

Another classical example is a second-order SM with a free parameter $\sigma \in \mathbb{R}$

$$\mathcal{S}_{\sigma\tau} \mathcal{S}_{(1-2\sigma)\tau} \mathcal{S}_{\sigma\tau} = e^{\frac{\sigma}{2}\tau A} e^{\sigma\tau B} e^{\frac{1-\sigma}{2}\tau A} e^{(1-2\sigma)\tau B} e^{\frac{1-\sigma}{2}\tau A} e^{\sigma\tau B} e^{\frac{\sigma}{2}\tau A},$$

which is promoted to the fourth-order SM $\mathcal{Y}_\tau$ (Yoshida) by requiring that [19, 33, 38]

$$2\sigma^3 + (1-2\sigma)^3 = 0 \quad \Rightarrow \quad \sigma = (2 + 2^{-1/3} + 2^{1/3})/3 \approx 1.35 \quad \Rightarrow \quad \ell(\mathcal{Y}_\tau) = O(\tau^5). \tag{6}$$

Note the appearance of negative time steps (via $\mathcal{S}_{(1-2\sigma)\tau}$ for the case at hand), which is an intrinsic property of all higher-order SMs [29, 34, 10]. The evolution backward in time makes parabolic problems ill-posed and imposes unnatural outflow boundary conditions upon hyperbolic problems. So much so, that even SMs with the complex-valued time steps (here with $\sigma \approx 0.32 \pm 0.13i$) may be preferable [34]. Modern computer-algebra yields effective methods to construct the higher-order SMs, see [12, 24, 11, 6, 4]. A comprehensive list of SMs, including those with complex time steps and SMs with $H = A + B + C$, can be found in [7].

A principle advantage of SMs is that a separate treatment of properly chosen partial flows is more efficient then the direct numerical approximation of the full problem. An example is given by the generalized nonlinear Schrödinger equation (GNLSE, see [1]) for a complex-valued wave envelope $u(t, x)$

$$i\frac{\partial}{\partial t} u(t,x) = \mathfrak{D}\left(-i\frac{\partial}{\partial x}\right) u(t,x) - \mathfrak{g}|u(t,x)|^2 u(t,x), \tag{7}$$

where the polynomial $\mathfrak{D}()$ relates the wave vector k and the frequency $\omega = \mathfrak{D}(k)$ of a linear modulation wave with $u \propto e^{i(kx-\omega t)}$. The parameter $\mathfrak{g}$ quantifies nonlinearity. A time-step for the GNLSE (7) is naturally split into the linear and nonlinear sub-steps

$$\begin{aligned} \frac{\partial}{\partial t} w_1(t,x) &= -i\mathfrak{D}\left(-i\frac{\partial}{\partial x}\right) w_1(t,x) \\ \frac{\partial}{\partial t} w_2(t,x) &= i\mathfrak{g}|w_2(t,x)|^2 w_2(t,x), \end{aligned} \tag{8}$$

cf., Eq. (2) and (3). The first sub-step can be addressed by the Fourier transform, the second equation is solved analytically because one can show that $|w_2(t,x)|$ is time-independent. For the time step selection strategy see [30].

Equation (7) will be used for numerical examples in what follows, whereas we note that SMs for GNLSE may be subject to numerical instabilities [37, 27]. To find $w_2(t)$ for a more sophisticated nonlinearity [1], one employs an ODE integrator, see [28, 17, 3]. Moreover, SMs based on Eq. (8) successfully apply to systems of coupled GNLSE-type equations [8], to GNLSE in several spatial dimensions [36], and to dissipative equations with complex-valued $\mathfrak{D}(k)$, see [21].

An important benefit of SMs is their ability to preserve certain intrinsic properties of the application-specific problem (1). For instance, the relation

$$u_1 = \mathcal{M}_\tau u_0 \quad \text{may imply} \quad u_0 = \mathcal{M}_{-\tau} u_1, \tag{9}$$

in which case the SM $\mathcal{M}_\tau$ supports time reversibility which is suitable for Hamiltonian problems. As to GNLSE, the SM for Eq. (8) preserves the L_2 norm of the solution, which is an important property of Eq. (7). The integral of motion is usually referred to as “energy” or “mass” or “particle number”.

Another principle advantage of SMs is that they can be adapted to parallel computing. In the first place, one picks H_m to enable parallel computation of the corresponding sub-step [26]. Aside from this, SMs can be run in parallel on standard PCs with multi-core processors even when the sub-steps do not enjoy such a property. Namely, the expression $e^{\tau H_M} \cdots e^{\tau H_2} e^{\tau H_1} u_0$ in Eq. (5) can simultaneously be calculated by several computer cores starting from the same u_0 but using a different order of the sub-steps [14, 16]. A weighted sum of the results may provide a better approximation of $u(\tau)$ than the individual SMs. The simplest example of such an additive scheme is given by the relation [32]

$$\frac{1}{2}\left(e^{\tau B} e^{\tau A} + e^{\tau A} e^{\tau B}\right) - e^{\tau(A+B)} = O(\tau^3), \tag{10}$$

where the first-order Lie-Trotter SM is promoted to a second-order additive SM (ASM). This is not a great improvement over the standard Strang splitting, however, ASMs can do much better than that.

The main result of this work is a new fourth-order ASM. The ASM is a weighted sum of four SMs with at most four exponential operators. Noteworthy, a generic SM with four exponents

$$\mathcal{M}_\tau = e^{b_2 \tau B} e^{a_2 \tau A} e^{b_1 \tau B} e^{a_1 \tau A},$$

has at best $\deg(\mathcal{M}_\tau) = 2$, which is achieved for a special (by a single free parameter) selection of the factors a_m and b_m, $m = 1, 2$, see [5]. On the other hand, the cubic and quartic terms in the Taylor expansion of $e^{\tau(A+B)}$ contain 20 mixed products. To promote from the second- to the fourth-order, we should take care of 20 coefficients and yet a proper combination of four SM provides $O(\tau^5)$ approximation of $e^{\tau(A+B)}$.

The paper is organized as follows. We start with a general discussion of the multiplicative SMs, give special attention to their symmetries, and calculate the local error of a SM derived from the seed one by a symmetry transformation. Then we turn to additive methods and study if and when an ASM performs better than the involved SMs. This information is used to construct useful ASMs by composing SMs, which are related to natural symmetries. We give a general rule and derive our ASM as a special case. Thereafter we discuss ASM’s local error, stability, and give numerical examples.

2 Multiplicative SMs

2.1 Definitions

Assume that the evolution Eq. (1) with $H = A + B$ is solved by a SM, the sub-steps are performed by alternating A and B, the first sub-step is performed with a multiple of A. A multiplicative SM $\mathcal{M}_\tau$ with s-stages is defined by two ordered sets of real or complex coefficients $a_{1\le m\le s}$ and $b_{1\le m\le s}$ such that

$$\mathcal{M}_\tau = e^{b_s\tau B}e^{a_s\tau A}\cdots e^{b_2\tau B}e^{a_2\tau A}e^{b_1\tau B}e^{a_1\tau A}, \quad \sum_{m=1}^{s} a_m = \sum_{m=1}^{s} b_m = 1, \tag{11}$$

where by construction $a_1 \neq 0$. It is natural to require that each inner exponential operator is not equal to the identity operator, still it may happen that $b_s = 0$. To cover SMs that employ B for the first sub-step, we also define a companion SM $\mathcal{M}_\tau^\circ$, where

$$\mathcal{M}_\tau^\circ = e^{b_s\tau A}e^{a_s\tau B}\cdots e^{b_2\tau A}e^{a_2\tau B}e^{b_1\tau A}e^{a_1\tau B}. \tag{12}$$

The upper index $\circ$ denotes swapping of A and B.

The number of the sequentially applied exponential operators is referred to as SM complexity

$$\rho(\mathcal{M}_\tau) = 2s \quad \text{for} \quad b_s \neq 0. \tag{13}$$

The SMs with $b_s = 0$, while employing $2s-1$ exponential operators, enjoy the FSAL (First Same As Last) property. We then use an effective complexity $\rho(\mathcal{M}_\tau) = 2s-2$, presupposing that evaluation of the intermediate solutions at every step can be spared. Complexity of an ASM is set to be the number of the exponential operators in the longest involved SM, e.g.,

$$\rho(\mathcal{L}_\tau) = \rho(\mathcal{S}_\tau) = \rho\left(\frac{1}{2}\mathcal{L}_\tau + \frac{1}{2}\mathcal{L}_\tau^\circ\right) = 2 \quad \text{and} \quad \rho\left(\frac{1}{2}\mathcal{S}_\tau + \frac{1}{2}\mathcal{S}_\tau^\circ\right) = 3,$$

because ASMs are always assumed to be calculated in parallel.

Any multiplicative SM $\mathcal{M}_\tau$ generates another important companion method

$$\mathcal{M}_\tau^\bullet = (\mathcal{M}_{-\tau})^{-1} = e^{a_1\tau A}e^{b_1\tau B}e^{a_2\tau A}e^{b_2\tau B}\cdots e^{a_s\tau A}e^{b_s\tau B}, \tag{14}$$

where $\mathcal{M}_\tau^\bullet$ results from reading of $\mathcal{M}_\tau$ from right to the left. The indices may be combined, e.g., $\mathcal{M}_\tau^{\circ\bullet}$ stands for $(\mathcal{M}_\tau^\circ)^\bullet$. Note, that

$$\mathcal{M}_\tau^{\circ\circ} = \mathcal{M}_\tau, \quad \mathcal{M}_\tau^{\bullet\bullet} = \mathcal{M}_\tau, \quad \mathcal{M}_\tau^{\circ\bullet} = \mathcal{M}_\tau^{\bullet\circ},$$
$$(\mathcal{M}_\tau\mathcal{N}_\tau)^\bullet = \mathcal{N}_\tau^\bullet\mathcal{M}_\tau^\bullet, \quad \text{but} \quad (\mathcal{M}_\tau\mathcal{N}_\tau)^\circ = \mathcal{M}_\tau^\circ\mathcal{N}_\tau^\circ.$$

A SM $\mathcal{P}_\tau$ is said to be palindromic, if

$$\mathcal{P}_\tau = \mathcal{P}_\tau^\bullet \quad \Rightarrow \quad \mathcal{P}_\tau\mathcal{P}_{-\tau} = \mathcal{P}_{-\tau}\mathcal{P}_\tau = \mathtt{I},$$

where $\mathtt{I}$ denotes the identity operator. Palindromic SMs, such as $\mathcal{S}_\tau$ and $\mathcal{Y}_\tau$, support time reversibility in the sense of Eq. (9). For a recent review on palindromic SMs see [15].

Actually one obtains up to $(2s)!/(s!)^2$ splittings by rearrangement of the exponents in Eq. (11). The transformations (12) and (14) are special because they provide new SMs without loss of accuracy: in the next Section we will demonstrate that $\deg(\mathcal{M}_\tau^\circ) = \deg(\mathcal{M}_\tau^\bullet) = \deg(\mathcal{M}_\tau)$. These SMs are then natural building blocks for an ASM. To proceed with this idea, we need more information on the local error structure.

2.2 Local error and discrepancy

If τ is small enough, any multiplicative SM $\mathcal{M}_\tau$ (11) can be presented in the form of a single exponential operator

$$\mathcal{M}_\tau = e^{b_s\tau B}e^{a_s\tau A}\cdots e^{b_2\tau B}e^{a_2\tau A}e^{b_1\tau B}e^{a_1\tau A} = e^{\tau(A+B)+\Delta(\mathcal{M}_\tau)}, \tag{15}$$

where $\Delta(\mathcal{M}_\tau)$ will be referred to as discrepancy of the operator $\mathcal{M}_\tau$. More precisely: using the fact that $\mathcal{M}_\tau \to \mathtt{I}$ for $\tau \to 0$, one can define $\ln \mathcal{M}_\tau$ by employing Taylor's expansion of $\ln(1+x)$ and then define

$$\Delta(\mathcal{M}_\tau) = \ln \mathcal{M}_\tau - (A+B)\tau,$$

at least for bounded A and B, see [23]. To derive an explicit expression for $\Delta(\mathcal{M}_\tau)$, we exploit the Baker-Campbell-Hausdorff (BCH) formula [22]

$$e^{\tau X}e^{\tau Y} = e^{\tau(X+Y)+\frac{\tau^2}{2}[X,Y]+\frac{\tau^3}{12}[X-Y,[X,Y]]-\frac{\tau^4}{24}[X,[Y,[X,Y]]]+\cdots}$$

with

$$[X_1, X_2] = X_1X_2 - X_2X_1.$$

The BCH formula is sequentially applied to the left-hand-side of Eq. (15) and implies the expression

$$\Delta(\mathcal{M}_\tau) = \sum_{q=2}^{\infty} \frac{[\mathcal{M}]_q}{q!}\tau^q, \tag{16}$$

where $[\mathcal{M}]_q$ denotes a certain linear combination of the basic commutators. The latter are listed in A and denoted by e_w, where w is a Lyndon word composed of A and B, see [9]. Each commutator within $[\mathcal{M}]_q$ is of length q and has a numerical factor that does not depend on τ, that is why index τ is omitted. Examples of the expansion (16) up to $q = 5$ are given in Table 1.

The local error of the SM $\mathcal{M}_\tau$ can be written as

$$\ell(\mathcal{M}_\tau) = \mathcal{M}_\tau - e^{\tau(A+B)} = e^{\tau(A+B)+\Delta(\mathcal{M}_\tau)} - e^{\tau(A+B)}. \tag{17}$$

Assuming that the discrepancy $\Delta(\mathcal{M}_\tau)$ is of order τ^{p+1} with $p \geq 1$, i.e., that the coefficients $[\mathcal{M}]_q$ in Eq. (16) vanish for $q \leq p$, we expand the right-hand-side of Eq. (17) with respect to τ and obtain

$$\begin{aligned}\ell(\mathcal{M}_\tau) = {} & \frac{[\mathcal{M}]_{p+1}}{(p+1)!}\tau^{p+1} + \left\{\frac{[\mathcal{M}]_{p+2}}{(p+2)!} + \frac{(A+B)\star[\mathcal{M}]_{p+1}}{2(p+1)!}\right\}\tau^{p+2} \\ & + \left\{\frac{[\mathcal{M}]_{p+3}}{(p+3)!} + \frac{(A+B)\star[\mathcal{M}]_{p+2}}{2(p+2)!} + \frac{(A+B)^2\star[\mathcal{M}]_{p+1}}{6(p+1)!} + \frac{\delta_{p1}}{2}\left(\frac{[\mathcal{M}]_{p+1}}{(p+1)!}\right)^2\right\}\tau^{p+3} \\ & + O(\tau^{p+4}).\end{aligned} \tag{18}$$

Here δ_{pq} denotes Kronecker delta and for the sake of brevity we use

$$X^n \star Y = X^nY + X^{n-1}YX + \cdots + YX^n,$$

for the sum of all possible products.

Equation (18) yields, that the orders of $\ell(\mathcal{M}_\tau)$ and $\Delta(\mathcal{M}_\tau)$ coincide and are equal to $p+1$, where $p = \deg(\mathcal{M}_\tau)$. Only the first term in Eq. (18) is of interest in the studies on multiplicative SMs. For our purposes, the full Eq. (18) is necessary, as we will see in the next Section.

Equation (16) contains all we need to know to compute discrepancies of the companion SMs derived from $\mathcal{M}_\tau$. We demonstrate this in three steps:

$\mathcal{M}$	$[\mathcal{M}]_2$	$[\mathcal{M}]_3$	$[\mathcal{M}]_4$	$[\mathcal{M}]_5$
$\mathcal{L}$	$-e_{AB}$	$\frac{1}{2}e_{AAB}+\frac{1}{2}e_{ABB}$	$-e_{AABB}$	$-\frac{1}{6}e_{AAAAB}+\frac{2}{3}e_{AAABB}+\frac{1}{3}e_{AABAB}+\frac{2}{3}e_{AABBB}+e_{ABABB}-\frac{1}{6}e_{ABBBB}$
$\mathcal{L}^\circ$	e_{AB}	$\frac{1}{2}e_{AAB}+\frac{1}{2}e_{ABB}$	e_{AABB}	$[\mathcal{L}^\circ]_5=[\mathcal{L}]_5$
$\mathcal{S}$	0	$-\frac{1}{4}e_{AAB}+\frac{1}{2}e_{ABB}$	0	$\frac{7}{48}e_{AAAAB}-\frac{7}{12}e_{AAABB}+\frac{1}{3}e_{AABAB}+\frac{2}{3}e_{AABBB}+e_{ABABB}-\frac{1}{6}e_{ABBBB}$
$\mathcal{S}^\circ$	0	$\frac{1}{2}e_{AAB}-\frac{1}{4}e_{ABB}$	0	$-\frac{1}{6}e_{AAAAB}+\frac{2}{3}e_{AAABB}+\frac{1}{3}e_{AABAB}-\frac{7}{12}e_{AABBB}-\frac{1}{4}e_{ABABB}+\frac{7}{48}e_{ABBBB}$

Table 1: Initial terms in the discrepancy expansion (16) for the classical SMs. Our notations for the basic commutators are explained in A. Note, that $\mathcal{L}^\bullet_\tau=\mathcal{L}^\circ_\tau$ and $\mathcal{S}^\bullet_\tau=\mathcal{S}_\tau$.

1 Swapping of A and B in Eq. (16) provides $\Delta(\mathcal{M}_\tau^\circ)$, where $[\mathcal{M}^\circ]_q = [\mathcal{M}]_q^\circ$. It is then obvious that $\deg(\mathcal{M}_\tau^\circ) = \deg(\mathcal{M}_\tau)$.

2 To calculate $\Delta(\mathcal{M}_\tau^\bullet)$, note that Eq. (14) yields $\mathcal{M}_\tau^\bullet \mathcal{M}_{-\tau} = \mathcal{M}_{-\tau}\mathcal{M}_\tau^\bullet = \mathtt{I}$, such that $\mathcal{M}_\tau^\bullet$ and $\mathcal{M}_{-\tau}$ commute. It follows that for any τ

$$\mathcal{M}_\tau^\bullet \mathcal{M}_{-\tau} = e^{(A+B)\tau+\Delta(\mathcal{M}_\tau^\bullet)} e^{-(A+B)\tau+\Delta(\mathcal{M}_{-\tau})} = e^{\Delta(\mathcal{M}_\tau^\bullet)+\Delta(\mathcal{M}_{-\tau})} = \mathtt{I}.$$

For a small enough τ we therefore obtain $\Delta(\mathcal{M}_\tau^\bullet) = -\Delta(\mathcal{M}_{-\tau})$ such that

$$[\mathcal{M}^\bullet]_q = (-1)^{q-1}[\mathcal{M}]_q \quad \text{and} \quad \deg(\mathcal{M}_\tau^\bullet) = \deg(\mathcal{M}_\tau). \tag{19}$$

Equation (19) has two further applications. First, we have the implication:

$$\text{if} \quad \mathcal{M}_\tau^\circ = \mathcal{M}_\tau^\bullet \quad \text{then} \quad [\mathcal{M}^\circ]_q = (-1)^{q-1}[\mathcal{M}]_q, \tag{20}$$

which directly applies to the Lie-Trotter SM in the second row of Table 1. Second, the discrepancy of a palindromic SM $\mathcal{P}_\tau$ must be an odd function of τ and $\deg(\mathcal{P}_\tau)$ must be an even number, because [38]

$$\mathcal{P}_\tau = \mathcal{P}_\tau^\bullet \quad \Rightarrow \quad \Delta(\mathcal{P}_\tau) = -\Delta(\mathcal{P}_{-\tau}) \quad \Rightarrow \quad [\mathcal{P}]_2 = [\mathcal{P}]_4 = [\mathcal{P}]_6 = \ldots = 0. \tag{21}$$

3 Last but not least, assume that a SM $\mathcal{M}_\tau$ is applied in two half-steps, e.g., to utilize Runge's rule. The discrepancy of the splitting $\mathcal{M}_\tau^/ = \mathcal{M}_{\tau/2}\mathcal{M}_{\tau/2}$ can be computed using Eq. (15) and taking into account that this time the exponents commute

$$\begin{aligned} e^{\tau(A+B)+\Delta(\mathcal{M}_{\tau/2}^2)} &= \mathcal{M}_{\tau/2}\mathcal{M}_{\tau/2} \\ &= e^{\frac{1}{2}\tau(A+B)+\Delta(\mathcal{M}_{\tau/2})} e^{\frac{1}{2}\tau(A+B)+\Delta(\mathcal{M}_{\tau/2})} = e^{\tau(A+B)+2\Delta(\mathcal{M}_{\tau/2})}, \end{aligned}$$

therefore $\Delta(\mathcal{M}_{\tau/2}^2) = 2\Delta(\mathcal{M}_{\tau/2})$ such that

$$[\mathcal{M}^/]_q = \frac{1}{2^{q-1}}[\mathcal{M}]_q \quad \text{and} \quad \deg(\mathcal{M}_\tau^/) = \deg(\mathcal{M}_\tau). \tag{22}$$

Altogether, Eq. (16) yields the following companion expansions

$$\Delta(\mathcal{M}_\tau^\circ) = \sum_{q=2}^{\infty} \frac{[\mathcal{M}]_q^\circ}{q!}\tau^q, \quad \Delta(\mathcal{M}_\tau^\bullet) = \sum_{q=2}^{\infty}(-1)^{q-1}\frac{[\mathcal{M}]_q}{q!}\tau^q, \quad \Delta(\mathcal{M}_\tau^/) = \sum_{q=2}^{\infty}\frac{[\mathcal{M}]_q}{2^{q-1}q!}\tau^q, \tag{23}$$

where actually all summations start from $q = \deg(\mathcal{M}_\tau) + 1$.

3 Additive methods

Additive methods will be denoted by bold calligraphic letters. A generic ASM $\boldsymbol{\mathcal{M}}_\tau$ is composed from $J \geq 2$ multiplicative SMs $\mathcal{M}_{j,\tau}$ via [26]

$$\boldsymbol{\mathcal{M}}_\tau = \sum_{j=1}^{J} c_j \mathcal{M}_{j,\tau} \quad \text{with} \quad \sum_{j=1}^{J} c_j = 1. \tag{24}$$

J is referred to as the number of independent threads to stress that ASMs are tailored for parallel computing [14]. Recall, that by definition ASM's complexity is $\rho(\boldsymbol{\mathcal{M}}_\tau) = \max_j \rho(\mathcal{M}_{j,\tau})$. The local error of a generic ASM is given by

$$\ell(\boldsymbol{\mathcal{M}}_\tau) = \boldsymbol{\mathcal{M}}_\tau - e^{\tau(A+B)} = \sum_{j=1}^{J} c_j(\mathcal{M}_{j,\tau} - e^{\tau(A+B)}) = \sum_{j=1}^{J} c_j \ell(\mathcal{M}_{j,\tau}), \tag{25}$$

where as above, the notation $\deg(\boldsymbol{\mathcal{M}}_\tau) = p$ indicates that $\ell(\boldsymbol{\mathcal{M}}_\tau) = O(\tau^{p+1})$. The multiplicative SMs in Eq. (24) may have different orders and we set

$$P = \min_{1\le j\le J} \deg(\mathcal{M}_{j,\tau}), \quad \bar{P} = \max_{1\le j\le J} \deg(\mathcal{M}_{j,\tau}).$$

We have $\deg(\boldsymbol{\mathcal{M}}_\tau) = P$ in the worst case. A useful ASM should advance beyond the best of the involved SMs. Therefore we would like to score $\deg(\boldsymbol{\mathcal{M}}_\tau) > \bar{P}$ by properly choosing c_j.

Equation (10) provides an example of the swap symmetrization [32]

$$\widetilde{\boldsymbol{\mathcal{L}}}_\tau = \frac{1}{2}\mathcal{L}_\tau + \frac{1}{2}\mathcal{L}_\tau^\circ, \quad P = \bar{P} = 1, \tag{26}$$

where $\deg(\widetilde{\boldsymbol{\mathcal{L}}}_\tau) = 2$. It is not a good idea to try

$$\widetilde{\boldsymbol{\mathcal{S}}}_\tau = \frac{1}{2}\mathcal{S}_\tau + \frac{1}{2}\mathcal{S}_\tau^\circ, \quad P = \bar{P} = 2, \tag{27}$$

because, as it happens, $\deg(\widetilde{\boldsymbol{\mathcal{S}}}_\tau) = 2$. Thus, swap symmetrization does not improve Strang's SM.

Burstein [14] suggested an ASM with four threads

$$\boldsymbol{\mathcal{B}}_\tau = \frac{4}{3}\widetilde{\boldsymbol{\mathcal{S}}}_\tau - \frac{1}{3}\widetilde{\boldsymbol{\mathcal{L}}}_\tau, \quad P = 1, \quad \bar{P} = 2, \tag{28}$$

where $\deg(\boldsymbol{\mathcal{B}}_\tau) = 3$. In what follows we are going to present a similar ASM but of fourth-order. To begin with we calculate the local error of a generic ASM.

3.1 Local error of additive methods

Equations (18) and (25) directly yield the expression for the local error of a generic ASM

$$\begin{aligned}\ell(\boldsymbol{\mathcal{M}}_\tau) = \frac{\sum c_j[\mathcal{M}_j]_{P+1}}{(P+1)!}\tau^{P+1} + \left\{\frac{\sum c_j[\mathcal{M}_j]_{P+2}}{(P+2)!} + \frac{(A+B)\star\sum c_j[\mathcal{M}_j]_{P+1}}{2(P+1)!}\right\}\tau^{P+2} \\ + \left\{\frac{\sum c_j[\mathcal{M}_j]_{P+3}}{(P+3)!} + \frac{(A+B)\star\sum c_j[\mathcal{M}_j]_{P+2}}{2(P+2)!} + \frac{(A+B)^2\star\sum c_j[\mathcal{M}_j]_{P+1}}{6(P+1)!}\right. \\ \left. + \frac{\delta_{P1}\sum c_j([\mathcal{M}_j]_{P+1})^2}{2(P+1)!(P+1)!}\right\}\tau^{P+3} + O(\tau^{P+4}),\end{aligned} \tag{29}$$

where all summations are over $1 \le j \le J$. Note, that even if a lucky choice of the weight coefficients yields that $\sum c_j[\mathcal{M}_j]_{P+1} = \sum c_j[\mathcal{M}_j]_{P+2} = \sum c_j[\mathcal{M}_j]_{P+3} = 0$, the local error may still be determined by $\sum c_j([\mathcal{M}_j]_{P+1})^2$. This happens with the Burstein ASM (28), where Eq. (29) and Table 1 yield that

$$\ell(\boldsymbol{\mathcal{B}}_\tau) = -\frac{\tau^4}{24}[A,B]^2 + O(\tau^5). \tag{30}$$

Further products of commutators, which are hidden in the $O(\tau^{P+4})$ term in Eq. (29), come into play if one tries to increase $\deg(\boldsymbol{\mathcal{M}}_\tau)$ beyond $P+3$.

Equation (29) implies to impose the restrictions

$$\begin{aligned}
&\sum_{j=1}^{J} c_j[\mathcal{M}_j]_{P+1} = 0,\\
&\sum_{j=1}^{J} c_j[\mathcal{M}_j]_{P+2} = 0,\\
&\sum_{j=1}^{J} c_j[\mathcal{M}_j]_{P+3} = 0 \;\;\&\&\;\; \delta_{P1}\sum_{j=1}^{J} c_j([\mathcal{M}_j]_{P+1})^2 = 0,\\
&\qquad\qquad \dots
\end{aligned} \tag{31}$$

where the first N conditions, if valid, promote $\deg(\boldsymbol{\mathcal{M}}_\tau)$ from the ab initio value P to $P+N$. We now apply Eq. (31) to derive ASMs with $P+N>\bar{P}$.

3.2 Richardson extrapolation

Consider Richardson extrapolation $\overline{\boldsymbol{\mathcal{M}}_\tau}$ of a generic SM $\mathcal{M}_\tau$

$$\overline{\boldsymbol{\mathcal{M}}_\tau} = c_1\mathcal{M}_\tau^{/} + c_2\mathcal{M}_\tau, \quad P=\bar{P}=\deg(\mathcal{M}_\tau), \quad c_1+c_2=1.$$

To increase $\deg(\overline{\boldsymbol{\mathcal{M}}_\tau})$ from P to $P+1$, we employ Eq. (22) and the first condition in (31)

$$\left(\frac{c_1}{2^P}+c_2\right)[\mathcal{M}]_{P+1}=0 \quad \Rightarrow \quad \frac{c_1}{2^P}+c_2=0,$$

because $\deg(\mathcal{M}_\tau)=P$ implies $[\mathcal{M}]_{P+1}\neq 0$. Solving the system of two linear equations for $c_{1,2}$, we get

$$c_1=\frac{2^P}{2^P-1}, \quad c_2=-\frac{1}{2^P-1}.$$

For instance, the simplest Lie-Trotter SM yields

$$\overline{\boldsymbol{\mathcal{L}}_\tau} = 2\mathcal{L}_\tau^{/} - \mathcal{L}_\tau \quad \text{with} \quad \deg(\overline{\boldsymbol{\mathcal{L}}_\tau})=2.$$

One may wish to get an ASM with positive weights like $\widetilde{\boldsymbol{\mathcal{L}}_\tau}$. To this end, consider

$$\widehat{\boldsymbol{\mathcal{M}}_\tau} = c_1\mathcal{M}_\tau^{/} + c_2\mathcal{M}_\tau^{\bullet}, \quad P=\bar{P}=\deg(\mathcal{M}_\tau), \quad c_1+c_2=1,$$

where Eq. (19) and (22) together with the first condition in (31) yield

$$c_1[\mathcal{M}^{/}]_{P+1} + c_2[\mathcal{M}^{\bullet}]_{P+1} = \left(\frac{c_1}{2^P}+(-1)^P c_2\right)[\mathcal{M}]_{P+1}=0 \quad \Rightarrow \quad \frac{c_1}{2^P}+(-1)^P c_2=0,$$

such that

$$c_1=\frac{2^P}{2^P+(-1)^{P+1}}, \quad c_2=\frac{(-1)^{P+1}}{2^P+(-1)^{P+1}}.$$

An odd $\deg(\mathcal{M}_\tau)$ provides then an ASM with positive weights, e.g.,

$$\widehat{\boldsymbol{\mathcal{L}}_\tau} = \frac{2}{3}\mathcal{L}_\tau^{/} + \frac{1}{3}\mathcal{L}_\tau^{\bullet} \quad \text{with} \quad \deg(\widehat{\boldsymbol{\mathcal{L}}_\tau})=2.$$

3.3 Richardson extrapolation of a palindromic SM

Consider a generic palindromic SM $\mathcal{P}_\tau$. A classical result [38] is that if $\deg(\mathcal{P}_\tau)$ increases by 1 by playing with the parameters a_m and b_m in Eq. (11), it actually increases by 2, because $\deg(\mathcal{P}_\tau)$ is an even number[1]. Now consider an ASM $\boldsymbol{\mathcal{P}}_\tau = \sum_{j=1}^{J} c_j \mathcal{P}_{j,\tau}$, which is composed from palindromic SMs. $\boldsymbol{\mathcal{P}}_\tau$ is not palindromic and still the classical result holds: if $\deg(\boldsymbol{\mathcal{P}}_\tau)$ increases by 1 by playing with c_j, it actually increases by 2.

Indeed, $P = \min_j \deg(\mathcal{P}_{j,\tau})$ must be an even number and therefore all $[\mathcal{P}_j]_{P+2} = 0$ due to Eq. (21). We see that Eq. (29) takes the form

$$\ell(\boldsymbol{\mathcal{P}}_\tau) = \frac{\sum c_j [\mathcal{P}_j]_{P+1}}{(P+1)!}\tau^{P+1} + \frac{(A+B)\star\sum c_j[\mathcal{P}_j]_{P+1}}{2(P+1)!}\tau^{P+2} + \left\{\frac{\sum c_j[\mathcal{P}_j]_{P+3}}{(P+3)!} + \frac{(A+B)^2\star\sum c_j[\mathcal{P}_j]_{P+1}}{6(P+1)!}\right\}\tau^{P+3} + \cdots,$$

where all summations are over $1 \le j \le J$. The first condition in Eq. (31) promotes then $\ell(\boldsymbol{\mathcal{P}}_\tau) = O(\tau^{P+1})$ directly to $\ell(\boldsymbol{\mathcal{P}}_\tau) = O(\tau^{P+3})$.

Corollary 1 *Richardson extrapolation of a palindromic method shall increase its order by 2.*

For instance, we have $\deg(\mathcal{S}_\tau) = 2$ and therefore obtain

$$\overline{\boldsymbol{\mathcal{S}}_\tau} = \widehat{\boldsymbol{\mathcal{S}}_\tau} = \frac{4}{3}\mathcal{S}^{/}_\tau - \frac{1}{3}\mathcal{S}_\tau \quad \text{with} \quad \deg(\overline{\boldsymbol{\mathcal{S}}_\tau}) = 4,$$

where the weights are calculated in the previous subsection. Note, that $\mathcal{S}^{/}_\tau$ contains five exponents and therefore $\rho(\overline{\boldsymbol{\mathcal{S}}_\tau}) = 5$, which is not a great improvement over $\mathcal{Y}_\tau$ with $\deg(\mathcal{Y}_\tau) = 4$ and an effective $\rho(\mathcal{Y}_\tau) = 6$. In the next subsection we derive a new ASM $\boldsymbol{\mathcal{N}}_\tau$ with $\deg(\boldsymbol{\mathcal{N}}_\tau) = 4$ and $\rho(\boldsymbol{\mathcal{N}}_\tau) = 4$.

3.4 The new ASM

We are now in a position to formulate the main result.

Theorem 1 *Let $\mathcal{M}_\tau$ be a SM for which $\deg(\mathcal{M}_\tau)$ is an odd number. Consider an ASM*

$$\boldsymbol{\mathcal{M}}_\tau = c_1\mathcal{M}_\tau + c_2\mathcal{M}^{\bullet}_\tau + c_3\mathcal{M}^{/}_\tau + c_4\mathcal{M}^{/\bullet}_\tau, \quad P = \bar{P} = \deg(\mathcal{M}_\tau), \tag{32}$$

$$c_1 + c_2 + c_3 + c_4 = 1. \tag{33}$$

Then a proper choice of the weight coefficients c_j provides $\deg(\boldsymbol{\mathcal{M}}_\tau) = P + 3$.

To proof the statement we note that the discrepancy expansions of all involved SMs are related to each other in accord with Eq. (23). To score $\deg(\boldsymbol{\mathcal{M}}_\tau) = P+3$ we need all conditions from Eq. (31),

[1] This is what promotes $\deg(\mathcal{S}_{\sigma\tau}\mathcal{S}_{(1-2\sigma)\tau}\mathcal{S}_{\sigma\tau}) = 2$ to $\deg(\mathcal{Y}_\tau) = 4$ for σ from Eq. (6).

which yields

$$\begin{aligned}
\left(c_1+(-1)^P c_2+\frac{c_3+(-1)^P c_4}{2^P}\right)[\mathcal{M}]_{P+1}=0,\\
\left(c_1+(-1)^P c_2+\frac{c_3+(-1)^P c_4}{2^{P+2}}\right)[\mathcal{M}]_{P+3}=0,\\
\left(c_1+(-1)^{P+1} c_2+\frac{c_3+(-1)^{P+1} c_4}{2^{P+1}}\right)[\mathcal{M}]_{P+2}=0,\\
\delta_{P1}\left(c_1+c_2+\frac{c_3+c_4}{2^{2P}}\right)([\mathcal{M}]_{P+1})^2=0.
\end{aligned} \tag{34}$$

The last equation can be ignored. It is a trivial identity for $P>1$ and it provides the same restriction upon c_j as the the equation above for $P=1$. The first two eqiuations yield $c_1+(-1)^P c_2=0$ and $c_3+(-1)^P c_4=0$ which, for an even P, violates Eq. (33). For an odd P, however, Eq. (33) and (34) are fulfilled by

$$c_1=c_2=-\frac{1}{2(2^{P+1}-1)},\quad c_3=c_4=\frac{2^P}{2^{P+1}-1},$$

which guarantees that $\deg(\boldsymbol{\mathcal{M}}_\tau)=P+3$.

For instance, the first-order Lie-Trotter SM generates the following new ASM

$$\boldsymbol{\mathcal{N}}_\tau=\frac{2}{3}\left(e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}+e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}\right)-\frac{1}{6}\left(e^{\tau B}e^{\tau A}+e^{\tau A}e^{\tau B}\right), \tag{35}$$

which shall be of fourth order. A direct calculation yields that

$$\begin{aligned}
\boldsymbol{\mathcal{N}}_\tau-e^{\tau(A+B)}=\frac{\tau^5}{120}\Bigg(&\frac{1}{24}e_{AAAAB}-\frac{1}{6}e_{AAABB}-\frac{1}{12}e_{AABAB}\\
&-\frac{1}{6}e_{AABBB}-\frac{1}{4}e_{ABABB}+\frac{1}{24}e_{ABBBB}\Bigg)+O(\tau^6),
\end{aligned}$$

where notations are explained in A.

Corollary 2 *Let $\mathcal{M}_\tau$ be a SM for which $\deg(\mathcal{M}_\tau)=P$ is an even number. The construction from Theorem 1 provides an ASM $\boldsymbol{\mathcal{M}}_\tau$ with $\deg(\boldsymbol{\mathcal{M}}_\tau)=P+2$.*

To proof we "downgrade" $\mathcal{M}_\tau$ by considering it as a SM of the odd order $P-1$. Thereafter Theorem 1 directly provides the desired ASM

$$\boldsymbol{\mathcal{M}}_\tau=\frac{2^{P-1}}{2^P-1}(\mathcal{M}'_\tau+\mathcal{M}'^{\bullet}_\tau)-\frac{1}{2(2^P-1)}(\mathcal{M}_\tau+\mathcal{M}^{\bullet}_\tau).$$

The result for even P is of less interest, because the improvement from P to $P+2$ is provided by, e.g., a more simple Richardson extrapolation of a palindromic SM.

3.5 Summary on splitting methods

For readers convenience, we provide Table 2 with all SMs and ASMs discussed above. For each method we give its order, an explicit definition, complexity ρ as in Eq. (13), number of threads J in accord with Eq. (24), and its local error estimate κ. The latter equals to the L_2 norm of the coefficients

determining the linear combination of basic commutators within the leading term of the local error ℓ. For the SMs of order p, we consider the coefficients of $[\mathcal{M}]_{p+1}$ in the case of multiplicative schemes, see Eq. (18), or $\sum c_j[\mathcal{M}_j]_{p+1}$ as in Eq. (29). The basis set of these combinations is given in A. Note, that products of commutators, like in Eq. (30), may spoil the standard definition of κ for an ASM. Last but not least, τ^I_{max} and τ^{II}_{max} are the largest possible time steps for a stable solution of two test examples, as discussed in the next Section.

4 Stability

4.1 A test problem

To get started we consider Eq. (1) with

$$u(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}, \quad H = A + B, \quad A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix},$$
$$e^{\tau H} = \begin{bmatrix} \cos\tau & \sin\tau \\ -\sin\tau & \cos\tau \end{bmatrix},$$

which corresponds to a harmonic oscillator addressed by the leapfrog method in [22]. The matrices of all SMs and ASMs from Table 2 can now be calculated explicitly. For example, we have

$$\mathcal{L}_\tau = e^{\tau B} e^{\tau A} = \begin{bmatrix} 1 & 0 \\ -\tau & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & \tau \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & \tau \\ -\tau & 1-\tau^2 \end{bmatrix}, \qquad \widetilde{\boldsymbol{\mathcal{L}}_\tau} = \begin{bmatrix} 1-\frac{1}{2}\tau^2 & \tau \\ -\tau & 1-\frac{1}{2}\tau^2 \end{bmatrix},$$

for the Lie-Trotter SM and its swap symmetrization respectively.

The simplest approach to the stability problem of the iteration procedure $u_{n+1} = \mathcal{M}_\tau u_n$ is to require that all eigenvalues λ_τ of $\mathcal{M}_\tau$ belong to the unit circle $|\lambda_\tau| \le 1$ in the complex plane. This typically leaves us with a stability interval $\tau \in [0, \tau_{\mathsf{max}}]$. For instance, one derives $\tau_{\mathsf{max}} = 2$ for the Lie-Trotter SM, which is then conditionally stable. Furthermore, we have $\det(\widetilde{\boldsymbol{\mathcal{L}}_\tau}) = 1 + \frac{1}{4}\tau^4$, such that the simplest ASM is unstable, no matter how small τ is.

A more comprehensive approach is to introduce a spectral norm $\|\mathcal{M}_\tau\|$ and to require that $\|\mathcal{M}_\tau\| \le 1$ which implies $\|u_{n+1}\| \le \|u_n\|$. To determine this norm, we are looking for the maximal (by modulus) eigenvalue of the symmetrized operator $(\mathcal{M}_\tau)^\dagger \mathcal{M}_\tau$. Here, $(\mathcal{M}_\tau)^\dagger$ denotes the adjoint operator. For instance, for the Lie-Trotter SM we have

$$(\mathcal{L}_\tau)^\dagger \mathcal{L}_\tau = \begin{bmatrix} 1+\tau^2 & \tau^3 \\ \tau^3 & 1-\tau^2+\tau^4 \end{bmatrix} \quad \Rightarrow \quad \|\mathcal{L}_\tau\| = 1 + \frac{1}{2}\tau^2 + O(\tau^4).$$

The condition $\|\mathcal{L}_\tau\| \le 1$ cannot be satisfied for $\tau \neq 0$. Of course, unstable methods may still be useful on a finite time interval, which is referred to as ρ-stability when $|\lambda_\tau| \le 1 + c\tau$.

We now consider the new ASM (35), where a direct calculation yields

$$\boldsymbol{\mathcal{N}}_\tau = \begin{bmatrix} 1-\frac{1}{2}\tau^2+\frac{1}{24}\tau^4 & \tau-\frac{1}{6}\tau^3 \\ -\tau+\frac{1}{6}\tau^3 & 1-\frac{1}{2}\tau^2+\frac{1}{24}\tau^4 \end{bmatrix} \qquad (\boldsymbol{\mathcal{N}}_\tau)^\dagger \boldsymbol{\mathcal{N}}_\tau = \left(1-\tfrac{1}{72}\tau^6+\tfrac{1}{576}\tau^8\right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

One can demonstrate that both approaches leave us with the same stability interval $\tau \in [0, 2\sqrt{2}]$.

Stability intervals of all SMs discussed in the manuscript are listed in the last two columns of Table 2 (see also Ref. [15]). One should stress that these results cover just one particular splitting of a simple test problem. With that in mind, both $\boldsymbol{\mathcal{B}}_\tau$ and $\boldsymbol{\mathcal{N}}_\tau$ have a clear advantage over the standard SMs.

$\mathcal{M}_\tau$	$\deg(\mathcal{M}_\tau)$	Definition	ρ	J	κ	$\tau^I_{\max}$	$\tau^{II}_{\max}$
$\mathcal{L}_\tau$	1	$e^{\tau B}e^{\tau A}$	2	1	1.0	2	0
$\widetilde{\boldsymbol{\mathcal{L}}_\tau}$	2	$\frac{1}{2}(e^{\tau B}e^{\tau A}+e^{\tau A}e^{\tau B})$	2	2	0.71	0	0
$\overline{\boldsymbol{\mathcal{L}}_\tau}$	2	$2e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}-e^{\tau B}e^{\tau A}$	4	2	0.35	2	2
$\widehat{\boldsymbol{\mathcal{L}}_\tau}$	2	$\frac{2}{3}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}+\frac{1}{3}e^{\tau A}e^{\tau B}$	4	2	0.35	0	0
$\mathcal{S}_\tau$	2	$e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}$	2	1	0.56	2	0
$\widetilde{\boldsymbol{\mathcal{S}}_\tau}$	2	$\frac{1}{2}(e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}+e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B})$	3	2	0.18	0	0
$\boldsymbol{\mathcal{B}}_\tau$	3	$\frac{2}{3}(e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}+e^{\frac{1}{2}\tau B}e^{\tau A}e^{\frac{1}{2}\tau B})-\frac{1}{6}(e^{\tau B}e^{\tau A}+e^{\tau A}e^{\tau B})$	3	4	NA	$\sqrt{3}$	$\sqrt{3}$
$\boldsymbol{\mathcal{N}}_\tau$	4	$\frac{2}{3}(e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}+e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B})-\frac{1}{6}(e^{\tau B}e^{\tau A}+e^{\tau A}e^{\tau B})$	4	4	0.36	$2\sqrt{2}$	$2\sqrt{2}$
$\overline{\boldsymbol{\mathcal{S}}_\tau}$	4	$\frac{4}{3}e^{\frac{1}{4}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{4}\tau B}e^{\frac{1}{4}\tau A}-\frac{1}{3}e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}$	5	2	0.35	2.59	0
$\mathcal{Y}_\tau$	4	$e^{\frac{\sigma}{2}\tau A}e^{\sigma\tau B}e^{\frac{1-\sigma}{2}\tau A}e^{(1-2\sigma)\tau B}e^{\frac{1-\sigma}{2}\tau A}e^{\sigma\tau B}e^{\frac{\sigma}{2}\tau A},\quad \sigma=\frac{2+2^{-1/3}+2^{1/3}}{3}$	6	1	3.35	1.57	0

Table 2: The table comprises all SMs and AMSs that are discussed in the manuscript. Splitting's order increases from top to bottom, methods with the same order are arranged by complexity. As it happens, $\kappa(\boldsymbol{\mathcal{B}}_\tau)$ does not make sense, see Eq. (30). The proposed ASM $\boldsymbol{\mathcal{N}}_\tau$ enjoys lower complexity (for a parallel evaluation) and much lower local error than the well-known $\mathcal{Y}_\tau$. The last two columns provide the stability intervals $\tau\in[0,\tau_{\max}]$ for two examples from the Section 4.

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4.2 General case

In the case of an arbitrary evolution operator H and its components H_m, we assume that the evolution problem (1) is solved on a finite time interval by applying small τ-steps and that all operators in the sequence (4) have exponential estimates

$$\|e^{\tau H_m}\| \le e^{\chi_m \tau} \quad \text{for} \quad \tau \ge 0 \quad \text{and some set} \quad \chi_m \in \mathbb{R}, \quad 1 \le m \le M. \tag{36}$$

We then have an iteration procedure

$$u_{n+1} = e^{\tau H_M} \cdots e^{\tau H_2} e^{\tau H_1} u_n \quad \text{with} \quad \|u_{n+1}\| \le e^{\chi\tau}\|u_n\|, \quad \chi = \sum_{m=1}^{M} \chi_m. \tag{37}$$

It is important to note that the estimate in Eq. (37) is valid for any rearrangement of the sub-steps $e^{\tau H_j}$, $j = 1, \ldots, M$. Moreover, the estimate remains valid for any ASM composed of such rearrangements with positive weights.

If $\chi \ge 0$, one expects ρ-stability of the SM (5), the latter applies on a finite time interval where the discrete solution converges to the exact one for $\tau \to 0$. If $\chi < 0$, the SM (5) is A-stable and is then formally safe to use for any $\tau > 0$. One may still face the problem of the numerical calculation of some operators $e^{\tau H_m}$ with $\chi_m > 0$. In practice, it might be desirable that each particular sub-step is A-stable such that all $\chi_m < 0$, the more so for nonlinear problems.

Whereas for a generic multiplicative SM $\mathcal{M}_\tau$ with $\deg(\mathcal{M}_\tau) > 2$ some of the coefficients $a_{1\le m\le s}$ and $b_{1\le m\le s}$ in Eq. (11) are negative [29, 34, 10], the most popular SMs with $\deg(\mathcal{M}_\tau) \le 2$, which are also used for construction of the additive SMs in Table 2, use only positive factors a_m and b_m. Just two estimates of the form

$$\|e^{\tau A}\| \le e^{\alpha\tau}, \quad \|e^{\tau B}\| \le e^{\beta\tau}, \quad \alpha, \beta \in \mathbb{R},$$

are then sufficient for achieving the estimate

$$\|\mathcal{M}_\tau\| = \|e^{b_s\tau B} e^{a_s\tau A} \cdots e^{b_1\tau B} e^{a_1\tau A}\| \le e^{(a_1+\cdots+a_s)\alpha\tau + (b_1+\cdots+b_s)\beta\tau} = e^{(\alpha+\beta)\tau},$$

and the same estimates for the SMs $\mathcal{M}^\circ_\tau$, $\mathcal{M}^\bullet_\tau$, and $\mathcal{M}^/_\tau$. Therefore the condition $\alpha + \beta < 0$ implies A-stability of the basic SM $\mathcal{M}_\tau$ and of all its companion SMs. Moreover, A-stability automatically applies to all ASMs composed of such SMs with only positive weights, e.g., to $\widetilde{\boldsymbol{\mathcal{L}}_\tau}$, $\widehat{\boldsymbol{\mathcal{L}}_\tau}$, and $\widetilde{\boldsymbol{\mathcal{S}}_\tau}$. The other ASMs from Table 2 require a separate consideration. For instance, we have

$$\|\overline{\boldsymbol{\mathcal{L}}_\tau}\| = \|2\mathcal{L}^/_\tau - \mathcal{L}_\tau\| \le \|\mathcal{L}^/_\tau\| + \|\mathcal{L}^/_\tau - \mathcal{L}_\tau\| = \|\mathcal{L}^/_\tau\| + \|\ell(\mathcal{L}^/_\tau) - \ell(\mathcal{L}_\tau)\| \le e^{(\alpha+\beta)\tau} + O(\tau^2).$$

and even for $\alpha + \beta < 0$ the condition $\|\overline{\boldsymbol{\mathcal{L}}_\tau}\| \le 1$ is only expected on some interval $\tau \in [0, \tau_{\mathsf{max}}]$.

5 Numerical examples

5.1 Problem formulation

In the rest of the manuscript we test performance of $\boldsymbol{\mathcal{N}}_\tau$ against the standard SMs from Table 2 in the framework of the GNLSE (7). Specifically, we consider several initial value problems for the

complex wave envelope $u(t,x)$ yielded by Eq. (7) with $0 \le t \le T$ and a proper initial condition $u(t,x)|_{t=0} = U(x)$. We assume that $u(t,x)$ is exponentially small outside a sufficiently large space interval $x \in [-\frac{X}{2}, \frac{X}{2}]$ to profit from an artificial periodic boundary condition at $x = \pm\frac{X}{2}$ and the discrete fast Fourier transform (DFFT) algorithms. The space interval is divided into N_x equal parts by introducing

$$\omega_h = \left\{ x_q = hq,\ h = \frac{X}{N_x},\ -\tfrac{1}{2}N_x \le q < \tfrac{1}{2}N_x \right\}, \quad u_q(t) = u(t,x_q), \quad u_q(0) = U(x_q), \quad (38)$$

with the corresponding discretization in the Fourier space

$$\left\{ k_p = \varkappa p,\ \varkappa = \frac{2\pi}{X},\ -\tfrac{1}{2}N_x \le p < \tfrac{1}{2}N_x \right\}, \quad u_p^F(t) = \frac{1}{N_x} \sum_{q=-N_x/2}^{N_x/2-1} u_q(t) e^{-ik_p x_q},$$

where

$$u_q(t) = \sum_{p=-N_x/2}^{N_x/2-1} u_p^F(t) e^{ik_p x_q} \quad \text{and} \quad \mathfrak{D}\left(-i\frac{\partial}{\partial x}\right) u(t,x)\Big|_{x=x_q} \approx \sum_{p=-N_x/2}^{N_x/2-1} \mathfrak{D}(k_p) u_p^F(t) e^{ik_p x_q}.$$

We are left with the semi-discrete version of the GNLSE (7) for $0 \le t \le T$

$$i\frac{d}{dt}u_q(t) = \sum_{p=-N_x/2}^{N_x/2-1} \mathfrak{D}(k_p) u_p^F(t) e^{ik_p x_q} - \mathfrak{g}|u_q(t)|^2 u_q(t), \quad -\frac{N_x}{2} \le q < \frac{N_x}{2} - 1. \quad (39)$$

The number N_x is taken large enough to neglect the spatial errors. The semi-discrete GNLSE is addressed using the splitting (8), where both sub-steps can be evaluated exactly (that is, up to rounding errors) and preserve L_2 norm of the solution. We use the same values of N_x and T for all methods from Table 2. The goal is to reveal how the solution depends on the time-step τ.

In general, we have no direct access to the exact solution of Eq.(39). Let's define the numerical error estimate ε as L_∞ norm of the difference of two numerical solutions at $t = T$

$$\varepsilon(\mathcal{M}_\tau, U, \omega_h, N_t) = \left\| (\mathcal{M}_\tau)^{N_t} U(\omega_h) - (\mathcal{M}_{\tau/10})^{10N_t} U(\omega_h) \right\|,$$

where $N_t = T/\tau$ is the number of the evolution steps and the vector $U(\omega_h)$ represents the initial condition. The solution with the reduced time-step $\tau/10$ is considered as the exact one. We investigate how ε decreases with τ and say that the SM shows the convergence rate r, if error's decay follows 2^{-r} rule when τ is reduced by half. Specifically, r is determined by applying the method of least-squares on $(\ln N_t, \ln \varepsilon)$ plane. The relation $r \approx \deg(\mathcal{M}_\tau)$ indicates that there are no unexpected error sources.

5.2 First-order soliton

We begin with the simulation of the first order soliton solution to Eq. (7) with $\mathfrak{D}(k) = \frac{1}{2}k^2$ and $\mathfrak{g} = 1$ and the initial condition $U(x) = \cosh^{-1}(x)$, see [2]. Values of the error estimate ε at $T = 10$ are given in Table 3 for different SMs and increasing N_t. The convergence rates, indicated in the bottom row of Table 3, agree with the theoretical SM orders from Table 2. We employ DFFT routines with a single-precision complex arithmetic, such that error scaling is not studied for the fourth order methods

	$\varepsilon(\mathcal{L}_\tau)$	$\varepsilon(\mathcal{S}_\tau)$	$\varepsilon(\overline{\boldsymbol{\mathcal{S}}_\tau})$	$\varepsilon(\mathcal{Y}_\tau)$	$\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$
$N_t = 40$			1.81664e-3	7.26833e-3	8.24797e-4
80			1.16498e-4	4.87016e-4	5.45073e-5
160	7.01606e-3	1.38238e-2	6.83105e-6	3.10562e-5	3.64076e-6
320	4.13420e-3	3.48481e-3	4.04148e-7	1.95132e-6	2.36680e-7
640	2.22680e-3	8.73054e-4	2.44113e-8	1.22152e-7	1.51068e-8
1280	1.15338e-3	2.18380e-4			
2560	5.87024e-4	5.46022e-5			
r	0.900	2.00	4.05	3.97	3.93

Table 3: Simulation errors for the first-order soliton solution of Eq. (7) with $\mathfrak{D}(k) = \frac{1}{2}k^2$ and $\mathfrak{g} = 1$. The bottom row provides the observed convergence rate. In all simulations we set $X = 40$, $N_x = 2^9$, and $T = 10$.

	$N_t = 200$	400	800	1600	3200	r
$\varepsilon(\mathcal{Y}_\tau)$	1.24473e-2	7.87660e-4	5.00139e-5	3.13807e-6	1.96365e-7	3.99
$\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$	1.42109e-4	5.15330e-5	4.75794e-6	3.46583e-7	2.34059e-8	3.24

Table 4: Simulation errors of the problem from Table 3 are calculated for $T = 40$.

and $N_t > 640$. The error estimates $\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$ and $\varepsilon(\overline{\boldsymbol{\mathcal{S}}_\tau})$ are $5 \div 10$ times smaller than $\varepsilon(\mathcal{Y}_\tau)$. This agrees with the local error estimates $\kappa(\boldsymbol{\mathcal{N}}_\tau) \approx \kappa(\overline{\boldsymbol{\mathcal{S}}_\tau}) \approx 0.1\kappa(\mathcal{Y}_\tau)$, see Table 2.

In addition, Table 4 compares $\varepsilon(\mathcal{Y}_\tau)$ to $\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$ for the same single-soliton solution but a larger $T = 40$. Both the scaling properties and the tenfold improvement of the SM error are preserved for $N_t > 800$. Such behaviour is less pronounced for $N_t < 800$, where the experimental convergence rate of the ASM $\boldsymbol{\mathcal{N}}_\tau$ was smaller than the theoretical value $\deg(\boldsymbol{\mathcal{N}}_\tau) = 4$. The reason is that the asymptotic convergence rates of the first-order SMs, which are composed together in Eq. (35), are not sufficiently resolved.

	$\varepsilon(\mathcal{L}_\tau)$	$\varepsilon(\mathcal{S}_\tau)$	$\varepsilon(\overline{\boldsymbol{\mathcal{S}}_\tau})$	$\varepsilon(\mathcal{Y}_\tau)$	$\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$
$N_t = 100$			3.69985e-2	4.47009e-2	7.15574e-3
200	1.08613e-1	1.83543e-1	2.24251e-3	3.45886e-3	3.94839e-4
400	4.25921e-2	4.71194e-2	1.09022e-4	2.28697e-4	2.29040e-5
800	1.83152e-3	1.18981e-2	5.54555e-6	1.44111e-5	1.60649e-6
1600	8.40914e-3	2.98237e-3	3.10452e-7	9.01738e-7	1.06730e-7
3200	4.01727e-3	7.46086e-4	1.85454e-8	5.64342e-8	6.91436e-9
r	1.19	1.99	4.21	3.93	3.98

Table 5: Simulation errors for the third-order soliton solution of Eq. (7) with $\mathfrak{D}(k) = \frac{1}{2}k^2$ and $\mathfrak{g} = 0.1$. In all simulations we set $X = 200$, $N_x = 2^{10}$, and $T = 20$.

	$\varepsilon(\mathcal{S}_\tau)$	$\varepsilon(\overline{\boldsymbol{\mathcal{S}}_\tau})$	$\varepsilon(\mathcal{Y}_\tau)$	$\varepsilon(\boldsymbol{\mathcal{N}}_\tau)$
$T = 40$				
$N_t = 200$	8.74539e-1	1.98626e-1	9.24272e-2	4.17667e-2
400	2.22850e-1	9.82089e-3	4.77576e-3	1.95076e-3
800	5.94293e-2	3.82992e-4	3.05633e-4	5.27988e-5
1600	1.52495e-2	1.50454e-5	1.92474e-5	9.49288e-7
3200	3.83895e-3	6.59972e-7	1.20438e-6	7.38628e-8
r	1.95	4.57	4.04	4.92
$T = 60$				
300	1.91689	2.0709e-1	1.37027e-1	4.71068e-2
600	5.21201e-1	9.86629e-3	9.62559e-3	1.89146e-3
1200	1.31805e-1	4.17595e-4	7.13351e-4	8.17543e-5
2400	3.30454e-2	1.82028e-5	3.86736e-5	3.62335e-6
4800	8.26508e-3	9.11710e-7	2.42040e-6	2.64053e-7
r	1.97	4.47	3.95	4.39
$T = 80$				
400	2.27782	9.93940e-1	2.96649e-1	2.06900e-1
800	4.47634e-1	3.86794e-2	1.43107e-2	9.50913e-3
1600	1.18411e-1	1.40593e-3	6.18969e-4	2.98742e-4
3200	3.06705e-2	5.01656e-5	3.86492e-5	7.04679e-6
6400	7.74153e-3	1.94427e-6	2.41869e-6	9.81209e-8
r	2.03	4.75	4.23	5.24

Table 6: Simulation errors of the problem from Table 5 for $T = 40$, 60, and 80.

5.3 Third-order soliton

Next, we have tested performance of the SMs by simulation of the evolution of a third-order soliton governed by the GNLSE (7) with $\mathfrak{D}(k) = \frac{1}{2}k^2$ and $\mathfrak{g} = 0.1$, see [2]. The initial condition is $U(x) = 1.89737\cosh^{-1}(x/5)$. To reduce the effect of the boundary conditions on a higher-order soliton, which tends to break up into fundamental solitons, we use a larger space domain, $X = 200$, and a larger number of the mesh points, $N_x = 2^{10}$. The errors are presented in Table 5. In all cases the convergence rate is similar to the order of the method, whereas the absolute error of $\boldsymbol{\mathcal{N}}_\tau$ is better than those of the other fourth-order methods.

As it was shown in, e.g., Ref. [2], the third-order soliton evolves periodically, with the period ≈ 40 for the case at hand. We therefore inspect the error estimate $\epsilon = \epsilon(t)$ for $T = 20,\ 40,\ 60,\ 80$ (Table 5 and three blocks of Table 6). The convergence rates of $\mathcal{S}_\tau$ and $\mathcal{Y}_\tau$ are in a good agreement with the the theoretical orders of the SMs. Moreover, both the convergence rate and the absolute error of the ASMs $\overline{\boldsymbol{\mathcal{S}}_\tau}$ and $\boldsymbol{\mathcal{N}}_\tau$, are better than expected, reaching $r > 5$ in the case of $\boldsymbol{\mathcal{N}}_\tau$ and $T = 80$. This welcome behaviour can be attributed to an unexpected cancellation of the local errors generated by the involved SMs. This cancellation requires further investigation.

5.4 Parallelization

To check applicability of the above SMs and ASMs to parallel computations, we provide several numerical tests for the problem of the third-order soliton from the previous section (Tables 5 and 6). We employ a fixed mesh with $X = 240$, $N_x = 2^{12}$, $T = 100$, and $N_t = 20000$. All simulations use a standard Intel® Core™ i7-6700 CPU processor with 4 cores, we employ an OpenMP library, which supports multi-platform shared memory multiprocessing programming.

We have used two parallelization strategies. The first strategy (S1) is tailored to a generic ASM (24). The involved SMs are calculated on J separate cores without an attempt to accelerate evaluation of the individual exponential operators. We consider two fourth-order ASMs, $\overline{\boldsymbol{\mathcal{S}}_\tau}$ with $J = 2$ and $\boldsymbol{\mathcal{N}}_\tau$ with $J = 4$. In the latter case we combine two smaller sub-problems into one job, to get a balanced distribution of tasks among 3 cores. No additional cost arise when implementing data communication because of the shared memory architecture.

The second strategy (S2) is tailored to a multiplicative SM, but can also be used for any ASM. All exponential operators are evaluated sequentially, we get use of the available computer cores when resolving "for" loops and executing DFFT algorithms. Note, that parallelization of the "for" loops, which are heavily exploited when resolving local nonlinear operators, is highly efficient, whereas parallelization of the DFFT involved in linear sub-problems is far from trivial. Still there are quite efficient parallel versions of DFFT algorithm for shared memory processors. We apply S2 to $\overline{\boldsymbol{\mathcal{S}}_\tau}$ and $\mathcal{Y}_\tau$. Of course, mixed strategies are also possible, as discussed below.

Table 7 provides calculation times for $\overline{\boldsymbol{\mathcal{S}}_\tau}$ (S1, S2), $\boldsymbol{\mathcal{N}}_\tau$ (S1) and $\mathcal{Y}_\tau$ (S2). There is no difference between S1 and S2 for a single core execution. The calculation time is mainly determined by the total number of the exponential operators. The new ASM $\boldsymbol{\mathcal{N}}_\tau$ with 12 such operators is then computationally most demanding, the ASM $\overline{\boldsymbol{\mathcal{S}}_\tau}$ with 8 operators is $\approx 35\%$ faster. The classical SM $\mathcal{Y}_\tau$, which involves 7 operators and enjoys FSAL property, performs even better. Two cores provide $\approx 35\%$ improvement for $\overline{\boldsymbol{\mathcal{S}}_\tau}$. Note that the involved sub-methods (Table 2) contain 5 and 3 exponential operators. i.e., the computational load is therefore differently distributed between the cores. The new ASM $\boldsymbol{\mathcal{N}}_\tau$ first comes into play for three cores and provides a similar load per core, because two less demanding sub-methods were executed on a single core. The parallel calculation is almost three times faster,

	$\overline{\boldsymbol{\mathcal{S}}_\tau}$ (S1)	$\boldsymbol{\mathcal{N}}_\tau$ (S1)	$\overline{\boldsymbol{\mathcal{S}}_\tau}$ (S2)	$\mathcal{Y}_\tau$ (S2)
#cores $= 1$	27.98	44.2	28.88	26.41
2	18.00		15.32	14.33
3		15.7	12.53	11.75
4			8.904	8.50

Table 7: Calculation times (in seconds) for parallel simulations of the third-order soliton problem on a fixed mesh $N_t \times N_x = 20000 \times 2^{12}$ with $T = 100$ employing S1 and S2 approaches.

	$N_t = 50$	100	200	400	r
$\mathcal{S}_\tau$	4.27453e-2	1.07951e-2	2.69881e-3	6.74393e-4	2.00
$\mathcal{Y}_\tau$	1.5508e-4	9.81039e-6	6.15523e-7	3.85115e-8	3.99
$\boldsymbol{\mathcal{N}}_\tau$	1.79263e-4	9.57609e-6	6.00006e-7	3.70988e-8	4.07

Table 8: Simulation errors for the Cherenkov radiation problem in the GNLSE with $\mathfrak{D}(k) = \frac{1}{2}k^2 - \frac{1}{6}k^3$ and $\mathfrak{g} = 1$. In all simulations we set $X = 400$, $N_x = 2^{12}$, and $T = 20$.

comparing to a single-core case.

The last two columns of Table 7 demonstrate that S2 provides a more significant acceleration of the calculations. Note, that the DFFT algorithm is very efficient when 2 or 4 (or 2^c) cores are used on a shared memory system, whereas the non-linear step welcomes any number of cores. We conclude that a generic ASM (24) favors use of $J \cdot 2^c$ cores and a mixed strategy. Namely, S2 applies to the sub-problems, which are assumed to have a good scaling up to 2^c cores. Thereafter S1 is used to combine the results. In the case of $\boldsymbol{\mathcal{N}}_\tau$, the use of $3 \cdot 2^c$ cores combines advantages of the relatively small local error estimate $\kappa(\boldsymbol{\mathcal{N}}_\tau)$ (Table 2) and fast calculation of the linear and nonlinear steps in the sub-problems. Note that like $\overline{\boldsymbol{\mathcal{S}}_\tau}$, our ASM $\boldsymbol{\mathcal{N}}_\tau$ can also use advantages of both strategies, S1 and S2, when $2 \cdot 2^c$ cores are available. In this case, to enjoy the balance of the computational load, we should use strategy S2 calculating each pair of longer ($\rho = 4$) and shorter ($\rho = 2$) sub-methods on 2^c cores. The challenge remains to develop efficient parallel SM schemes for global memory supercomputers and clusters of processors.

5.5 Simulation of more general GNLS problem

In the above examples we have studied solitons of Eq. (7) with $\mathfrak{D}(k) = \frac{1}{2}k^2$, which is integrable, that is why analytical solutions for the fundamental and higher-order solitons are available [2]. Here we consider a non-integrable GNLSE with $\mathfrak{D}(k) = \frac{1}{2}k^2 - \frac{1}{6}k^3$ and $\mathfrak{g} = 1$, the initial condition reads $U(x) = 1.58114\cosh^{-1}(x/2)$. The corresponding semi-discrete system (39) is solved for $X = 400$, $N_x = 2^{12}$, and $T = 40$ by splitting into linear and non-linear sub-problems as in Eq. (8). The initial pulse evolves producing the so called Cherenkow radiation [18]. We calculate pulse evolution and compare performance of the new SM $\boldsymbol{\mathcal{N}}_\tau$ with that one of widely used Strang's and Yoshida's methods $\mathcal{S}_\tau$ and $\mathcal{Y}_\tau$, see [3] for application of other SMs. The numerical test results collected in Table 8 show, that the application of $\boldsymbol{\mathcal{N}}_\tau$ preserves the fourth-order convergence rate and provides the errors which are very similar to those obtained by Yoshida's method.

6 Conclusions

Our result is that a generic splitting method of order P can be used to generate three companion splitting methods of the same order and finally to construct an additive splitting method of order $P+3$. The weight coefficients depend only on P, which must be an odd number. If the seed method contains S exponential operators, the additive method contains $2S + 2S + S + S = 6S$ operators, which can be calculated in parallel. Namely, $2S$ operators correspond to the first independent thread, $2S$ to the second, and two methods with S operators can be combined into the third thread. An natural application of our approach is when parallel evaluation of the seed splitting method shows good scaling for up to C cores. One can then employ $3C$ cores with our additive method to improve the seed method's order by 3. Additional costs are negligible on a system with the shared memory.

A Basis commutators

For the first- and second-order methods we use the following basic commutators

$$e_{AB} = [A, B], \qquad e_{AAB} = [A, [A, B]], \qquad e_{ABB} = [[A, B], B].$$

More specifically, one profits from a one-to-one correspondence $w \mapsto e_w$ between the Lyndon words w (composed of "letters" A and B in accord with the special rules) and linearly independent basic commutators e_w, see [9]. For instance, the local error for all methods with $p = 3$ is spanned by the set

$$e_{AAAB} = [A, [A, [A, B]]], \qquad e_{AABB} = [A, [[A, B], B]], \qquad e_{ABBB} = [[[A, B], B], B],$$

where relations like $[A, [[A, B], B]] = [[A, [A, B]], B]$ reduce the total number of independent basic commutators, which reflects the existence of the so-called generalized Jacobi identities [13]. For $p = 4$ the basis consists of six commutators

$$\begin{aligned} e_{AAAAB} &= [A, [A, [A, [A, B]]]], & e_{AAABB} &= [A, [A, [[A, B], B]]], \\ e_{AABAB} &= [[A, [A, B]], [A, B]], & e_{AABBB} &= [A, [[[A, B], B], B]], \\ e_{ABABB} &= [[A, B], [[A, B], B]], & e_{ABBBB} &= [[[[A, B], B], B], B], \end{aligned}$$

where a lexicographical order of the corresponding Lyndon words is used.

Note, that swapping of A and B is applied to the basic commutators when $\Delta(\mathcal{M}^\circ_\tau)$ is calculated from Eq. (23) in which case we have

$$e^\circ_{AB} = -e_{AB}, \quad e^\circ_{AAB} = e_{ABB}, \quad e^\circ_{AAAB} = e_{ABBB}, \quad e^\circ_{AABB} = -e_{AABB}, \quad \text{etc.}$$

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