Additive splitting methods for parallel solutions of evolution problems

R. Čiegis

Vilnius Gediminas Technical University, Vilnius, Lithuania
e-mail: rc@vgtu.lt

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Kurt Busch (Max Planck institute Berlin, Germany)

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Abstract

We demonstrate how a multiplicative splitting method of order P can be utilized 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 of a test problem, and numerical examples with special discussion of the parallelization properties and applications to nonlinear optics.

Introduction

Consider an abstract initial value problem within a sufficiently short evolution step τ

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

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

The final state $u(\tau)$ of the the evolution problem (1) is approximated following the sequence

$$u_0 \xrightarrow{e^{\tau H_1}} w_1(\tau) \xrightarrow{e^{\tau H_2}} w_2(\tau) \xrightarrow{e^{\tau H_3}} \cdots \xrightarrow{e^{\tau H_{M-1}}} w_{M-1}(\tau) \xrightarrow{e^{\tau H_M}} w_M(\tau), \tag{2}$$

where $w_1(\tau)$ is calculated by solving the sub-problem

$$\frac{d}{dt} w_1(t) = H_1 w_1(t), \quad w_1(0) = u_0, \quad t \in [0, \tau], \tag{3}$$

followed by the calculation of $w_2(\tau)$,

$$\frac{d}{dt} w_2(t) = H_2 w_2(t), \quad w_2(0) = w_1(\tau), \quad t \in [0, \tau], \tag{4}$$

etc. The last member $w_M(\tau)$ approximates $u(\tau)$.

Generally, the components H_m do not commute, they can be applied in different order.

The local error of a given SM can be characterized 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 local error estimate follows from the Taylor expansion if all components of H are bounded.

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

$$\mathcal{L}_\tau = e^{\tau B} e^{\tau A} \quad \text{with} \quad \ell(\mathcal{L}_\tau) = e^{\tau B} e^{\tau A} - e^{\tau(A+B)} = O(\tau^2). \quad (5)$$

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

$$\mathcal{S}_\tau = e^{\frac{1}{2}\tau A} e^{\tau B} e^{\frac{1}{2}\tau A} \quad \text{with} \quad \ell(\mathcal{S}_\tau) = O(\tau^3). \quad (6)$$

Another example is a “cascaded” second-order SM with a free parameter σ

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

It is promoted to the classical fourth-order SM $\mathcal{Y}_\tau$ (Yoshida), for a special σ.

An example is given by the generalized nonlinear Schrdinger equationn (GNLSE) for a complex-valued wave envelope $u(t,x)$

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

where the polynomial $\mathfrak{D}()$ relates the wave vector k and the frequency $\omega = \mathfrak{D}(k)$ of a linear modulation wave. One time step for the GNLSE is naturally split into the linear and nonlinear sub-steps

$$\frac{\partial}{\partial t}w_1(t,x) = -i\mathfrak{D}\left(-i\frac{\partial}{\partial x}\right)w_1(t,x),$$
$$\frac{\partial}{\partial t}w_2(t,x) = i\mathfrak{g}|w_2(t,x)|^2 w_2(t,x).$$

Multiplicative SMs

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

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

$$\sum_{m=1}^{s} a_m = \sum_{m=1}^{s} b_m = 1,$$

We also define a companion SM $\mathcal{M}_\tau^\circ$, where the upper index $\circ$ denotes swapping of A and B

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

$$(\mathcal{M}_\tau \mathcal{N}_\tau)^\circ = \mathcal{M}_\tau^\circ \mathcal{N}_\tau^\circ.$$

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

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

$$(\mathcal{M}_\tau \mathcal{N}_\tau)^\bullet = \mathcal{N}_\tau^\bullet \mathcal{M}_\tau^\bullet.$$

Local error and discrepancy

If τ is small enough, any multiplicative SM can be transformed to a single exponential operator

$$e^{b_s \tau B} e^{a_s \tau A} \cdots e^{b_2 \tau B} e^{a_2 \tau A} e^{b_1 \tau B} e^{a_1 \tau A} = \mathcal{M}_\tau = e^{\tau(A+B)+\Delta(\mathcal{M}_\tau)}, \tag{8}$$

where $\Delta(\mathcal{M}_\tau)$ will be referred to as discrepancy of the operator $\mathcal{M}_\tau$.
To derive an explicit expression for $\Delta(\mathcal{M}_\tau)$, we exploit the Baker-Campbell-Hausdorff (BCH) formula

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

with $[X_1, X_2] = X_1 X_2 - X_2 X_1$.

The BCH formula is sequentially applied to the left-hand-side of Eq. (8) and implies the expression

$$\Delta(\mathcal{M}_\tau) = \sum_{q=2}^{\infty} \frac{[\mathcal{M}]_q}{q!} \tau^q, \tag{9}$$

where $[\mathcal{M}]_q$ denotes a certain linear combination of the basis commutators.

Equation (9) contains all we need to know to compute discrepancies of the companion SMs derived from $\mathcal{M}_\tau$.

Additive methods

A generic ASM $\boldsymbol{\mathcal{M}}_\tau$ is composed from $J \geq 2$ multiplicative SMs $\mathcal{M}_{j,\tau}$ via

$$\boldsymbol{\mathcal{M}}_\tau = \sum_{j=1}^{J} c_j \mathcal{M}_{j,\tau} \quad \text{with} \quad \sum_{j=1}^{J} c_j = 1. \tag{10}$$

Parallelization is here!

The local error of a generic ASM is given by

$$\ell(\boldsymbol{\mathcal{M}}_\tau) = \boldsymbol{\mathcal{M}}_\tau - e^{\tau(A+B)} = \sum_{j=1}^{J} c_j (\mathcal{M}_{j,\tau} - e^{\tau(A+B)}) = \sum_{j=1}^{J} c_j \ell(\mathcal{M}_{j,\tau}), \tag{11}$$

The multiplicative SMs in Eq. (10) 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 want to construct new ASMs, such that

$$\deg(\boldsymbol{\mathcal{M}}_{\mathbf{j},\boldsymbol{\tau}}) > \bar{P}.$$

Examples

1.

$$\widetilde{\boldsymbol{\mathcal{L}}}_\tau = \frac{1}{2}\mathcal{L}_\tau + \frac{1}{2}\mathcal{L}^\circ_\tau, \quad P = \bar{P} = 1, \tag{12}$$

where $\deg(\widetilde{\boldsymbol{\mathcal{L}}}_\tau) = 2$.

2.
It is not a good idea to try

$$\widetilde{\boldsymbol{\mathcal{S}}}_\tau = \frac{1}{2}\mathcal{S}_\tau + \frac{1}{2}\mathcal{S}^\circ_\tau, \quad P = \bar{P} = 2, \tag{13}$$

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

3.

Burstein and Mirin suggested an ASM with four threads

$$\mathcal{B}_\tau = \frac{4}{3}\widetilde{\mathcal{S}_\tau} - \frac{1}{3}\widetilde{\mathcal{L}_\tau}, \quad P = 1, \quad \bar{P} = 2, \tag{14}$$

where $\deg(\mathcal{B}_\tau) = 3$.

The local error of a generic ASM can be written as

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

Richardson extrapolation

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

$$\overline{\boldsymbol{\mathcal{M}}_\tau} = \frac{2^P \mathcal{M}_\tau^{/} - \mathcal{M}_\tau}{2^P - 1}.$$

For instance, $\deg(\mathcal{L}_\tau) = 1$ provides $\overline{\boldsymbol{\mathcal{L}}_\tau} = 2\mathcal{L}_\tau^{/} - \mathcal{L}_\tau$ with $\deg(\overline{\boldsymbol{\mathcal{L}}_\tau}) = 2$.

Richardson extrapolation of a palindromic SM

Consider a generic palindromic SM $\mathcal{P}_\tau$. A classical result is that if $\deg(\mathcal{P}_\tau)$ increases by 1 by playing with the parameters a_m and b_m in ASM equations, it actually increases by 2, because $\deg(\mathcal{P}_\tau)$ is an even number.

Theorem

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 we use the expressions for weights from the previous subsection.

The main result

Theorem

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

$$\boldsymbol{\mathcal{M}}_\tau = c_1\mathcal{M}_\tau + c_2\mathcal{M}_\tau^{\bullet} + c_3\mathcal{M}_\tau^{/} + c_4\mathcal{M}_\tau^{/\bullet}, \quad P = \bar{P} = \deg(\mathcal{M}_\tau),$$
$$c_1 + c_2 + c_3 + c_4 = 1.$$

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

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

$$\mathcal{N}_\tau = \frac{2}{3}\left(e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A} + e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B}\right) - \frac{1}{6}\left(e^{\tau B}e^{\tau A} + e^{\tau A}e^{\tau B}\right), \tag{15}$$

Stability

Motivated by the concept of A-stability for ordinary differential equations, we consider the problem

$$\frac{d}{dt}z(t) = \lambda z(t), \quad \lambda \in \mathbb{C}, \quad \mathrm{Re}(\lambda) < 0. \tag{16}$$

The problem is adapted to our framework by setting $z = x + iy$ with

$$u(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}, \qquad H = A + B,$$
$$A = \begin{bmatrix} \mathrm{Re}(\lambda) & -\mathrm{Im}(\lambda) \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ \mathrm{Im}(\lambda) & \mathrm{Re}(\lambda) \end{bmatrix},$$

Examples are shown in Fig. 1, we also indicate subdomains where A-stable SMs are contractive, such that

$$u_{n+1} = \mathcal{M}_\tau u_n$$

implies $\|u_{n+1}\| < \|u_n\|$ for the L_2 norm. All considered schemes are only conditionally stable, but the stability domain of the ASM $\mathcal{N}_\tau$ is the largest.

We also note that Yoshida's SM is not recommended for a large dissipation, e.g., when the spectrum of an optical pulse expands beyond the transparency window of a fiber.

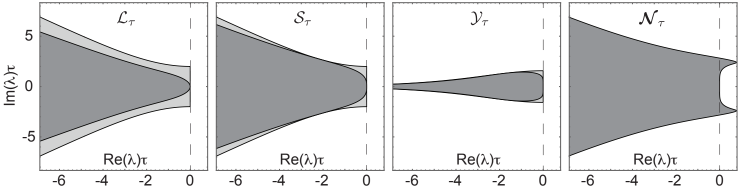

FIGURE : Stability domains of the standard SMs and the proposed ASM for the test problem (16). Light gray indicates A-stability, in gray domains SMs are A-stable and, moreover, contractive. A-stable domains for $\mathcal{L}_\tau$ and $\mathcal{S}_\tau$ are identical. Abnormal behavior of $\mathcal{Y}_\tau$ with the increase of dissipation is related to the negative time step $(1 - 2\sigma_0)\tau$. Light gray and gray domains are the same for the new ASM.

Numerical Experiments

Simulation errors ε versus the number of time steps N_t for the soliton solutions of Eq. (7) with $\mathfrak{D}(k) = k^2/2$.

The calculation results (points) are shown from top to bottom for $\mathcal{L}_\tau$ (gray), $\mathcal{S}_\tau$ (black), $\boldsymbol{\mathcal{B}}_\tau$ (brown), $\mathcal{Y}_\tau$ (blue), $\boldsymbol{\mathcal{N}}_\tau$ (red), and $\overline{\boldsymbol{\mathcal{S}}}_\tau$ (green). Straight lines correspond to the optimal fit $\varepsilon = C\tau^p$. For the first-order soliton in (a,b) we set $\mathfrak{g} = 1$, $X = 40$, $N_x = 2^9$ and either $T = 10$ (a) or $T = 40$ (b).

For the third-order soliton in (c,d) we set $\mathfrak{g} = 0.1$, $X = 200$, $N_x = 2^{10}$ and either $T = 20$ (c) or $T = 100$ (d).

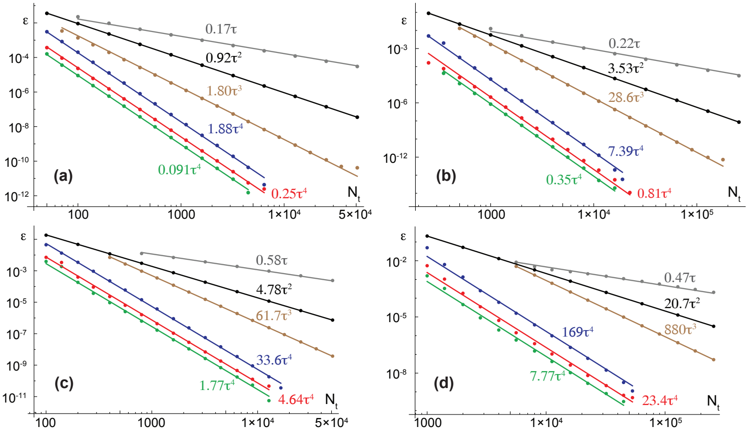

FIGURE : Simulation errors ε versus the number of time steps N_t for the soliton solutions of Eq. (7) with $\mathfrak{D}(k) = k^2/2$.