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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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.
Consider an abstract initial value problem within a sufficiently short evolution step $\tau$

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

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 $du/dt = H_mu$ can easily be addressed and generate individual semigroups.
The final state $u(\tau)$ of the evolution problem (1) is approximated following the sequence

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

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 $S_\tau$, reads

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

Another example is a “cascaded” second-order SM with a free parameter $\sigma$

$$C_{\sigma,\tau} = S_{\sigma \tau} S_{(1-2\sigma)\tau} S_{\sigma \tau} = e^{\frac{\sigma}{2} \tau A} e^{\sigma \tau B} e^{\frac{1-\sigma}{2} \tau A} e^{(1-2\sigma)\tau B} e^{\frac{1-\sigma}{2} \tau A} e^{\sigma \tau B} e^{\frac{\sigma}{2} \tau A}.$$ 

It is promoted to the classical fourth-order SM $\mathcal{Y}_\tau$ (Yoshida), for a special $\sigma$. 
An example is given by the generalized nonlinear Schrödinger equation (GNLSE) for a complex-valued wave envelope $u(t, x)$

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

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

$$\frac{\partial}{\partial t} w_1(t, x) = -i \mathcal{D} \left( -i \frac{\partial}{\partial x} \right) w_1(t, x),$$

$$\frac{\partial}{\partial t} w_2(t, x) = ig |w_2(t, x)|^2 w_2(t, x).$$
A multiplicative SM $M_{\tau}$ with $s$-stages is defined by two ordered sets of real or complex coefficients $a_1 \leq m \leq s$ and $b_1 \leq m \leq s$ such that

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

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

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

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

$$(M_{\tau} N_{\tau})^{\circ} = M^{\circ}_{\tau} N^{\circ}_{\tau}.$$
Any multiplicative SM $M_\tau$ generates another important companion method

$$M^\bullet_\tau = (M_{-\tau})^{-1} = e^{a_1 \tau A} e^{b_1 \tau B} e^{a_2 \tau A} e^{b_2 \tau B} \ldots e^{a_s \tau A} e^{b_s \tau B},$$

$$(M_\tau N_\tau)^\bullet = N_\tau^\bullet M_\tau.$$
If $\tau$ is small enough, any multiplicative SM can be transformed to a single exponential operator

$$e^{b_s \tau B} e^{a_s \tau A} \ldots e^{b_2 \tau B} e^{a_2 \tau A} e^{b_1 \tau B} e^{a_1 \tau A} = M_\tau = e^{\tau (A+B) + \Delta (M_\tau)},$$

where $\Delta (M_\tau)$ will be referred to as discrepancy of the operator $M_\tau$.

To derive an explicit expression for $\Delta (M_\tau)$, we exploit the Baker-Campbell-Hausdorff (BCH) formula

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

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

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

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

$$\mathcal{M}_\tau = \sum_{j=1}^{J} c_j \mathcal{M}_{j,\tau} \quad \text{with} \quad \sum_{j=1}^{J} c_j = 1.$$  \hspace{1cm} (10)

Parallelization is here!

The local error of a generic ASM is given by

$$\ell(\mathcal{M}_\tau) = \mathcal{M}_\tau - e^{\tau(A+B)} = \sum_{j=1}^{J} c_j (\mathcal{M}_{j,\tau} - e^{\tau(A+B)}) = \sum_{j=1}^{J} c_j \ell(\mathcal{M}_{j,\tau}),$$ \hspace{1cm} (11)
The multiplicative SMs in Eq. (10) may have different orders and we set

\[ P = \min_{1 \leq j \leq J} \deg(M_{j, \tau}), \quad \bar{P} = \max_{1 \leq j \leq J} \deg(M_{j, \tau}). \]

We want to construct new ASMs, such that

\[ \deg(M_{j, \tau}) > \bar{P}. \]
Examples

1. 
\[ \widetilde{L}_\tau = \frac{1}{2}L_\tau + \frac{1}{2}L^\circ_\tau, \quad P = \bar{P} = 1, \] 
(12) 
where \( \deg(\widetilde{L}_\tau) = 2. \)

2. 
It is not a good idea to try 
\[ \widetilde{S}_\tau = \frac{1}{2}S_\tau + \frac{1}{2}S^\circ_\tau, \quad P = \bar{P} = 2, \] 
(13) 
because \( \deg(\widetilde{S}_\tau) = 2. \) Thus, swap symmetrization does not improve Strang’s SM.
3.

Burstein and Mirin suggested an ASM with four threads

\[ \mathcal{B}_\tau = \frac{4}{3} \mathcal{S}_\tau - \frac{1}{3} \mathcal{L}_\tau, \quad P = 1, \quad \bar{P} = 2, \]  

where \( \text{deg}(\mathcal{B}_\tau) = 3. \)
The local error of a generic ASM can be written as

$$\ell(\mathcal{M}_\tau) = \frac{\sum c_j [\mathcal{M}_j]_{P+1}}{(P+1)!} \tau^{P+1} + \left\{ \frac{\sum c_j [\mathcal{M}_j]_{P+2}}{(P+2)!} + \frac{(A+B) \times \sum c_j [\mathcal{M}_j]_{P+1}}{2(P+1)!} \right\} \tau^{P+2}$$

$$+ \left\{ \frac{\sum c_j [\mathcal{M}_j]_{P+3}}{(P+3)!} + \frac{(A+B) \times \sum c_j [\mathcal{M}_j]_{P+2}}{2(P+2)!} \right\} \tau^{P+3} + O(\tau^{P+4}).$$
Consider Richardson extrapolation $\overline{M}_\tau$ of a generic SM $M_\tau$

$$\overline{M}_\tau = \frac{2^p M'_\tau - M_\tau}{2^p - 1}.$$ 

For instance, $\deg(L_\tau) = 1$ provides $\overline{L}_\tau = 2L'_\tau - L_\tau$ with $\deg(\overline{L}_\tau) = 2$. 
Richardson extrapolation of a palindromic SM

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

**Theorem**

*Richardson extrapolation of a palindromic method shall increase its order by 2.*
For instance, we have \( \text{deg}(S\tau) = 2 \) and therefore obtain

\[
\overline{S}\tau = \hat{S}_{\tau} = \frac{4}{3} S'_{\tau} - \frac{1}{3} S_{\tau}
\]

with \( \text{deg}(\overline{S}_{\tau}) = 4 \),

where we use the expressions for weights from the previous subsection.
THE MAIN RESULT

THEOREM

Let $M_\tau$ be a SM for which $\deg(M_\tau)$ is an odd number. Consider an ASM

$$M_\tau = c_1 M_\tau + c_2 M_\tau^\bullet + c_3 M_\tau^/ + c_4 M_\tau^/\bullet, \quad P = \tilde{P} = \deg(M_\tau),$$

$$c_1 + c_2 + c_3 + c_4 = 1.$$

Then a proper choice of the weight coefficients $c_j$ provides $\deg(M_\tau) = P + 3$. 
For instance, the first-order Lie-Trotter SM generates the following new ASM

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

(15)
Motivated by the concept of A-stability for ordinary differential equations, we consider the problem

\[ \frac{d}{dt} z(t) = \lambda z(t), \quad \lambda \in \mathbb{C}, \quad \text{Re}(\lambda) < 0. \] (16)

The problem is adapted to our framework by setting \( z = x + iy \) with

\[ u(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}, \quad H = A + B, \]

\[ A = \begin{bmatrix} \text{Re}(\lambda) & -\text{Im}(\lambda) \\ 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ \text{Im}(\lambda) & \text{Re}(\lambda) \end{bmatrix}. \]
Examples are shown in Fig. 1, we also indicate subdomains where A-stable SMs are contractive, such that

$$u_{n+1} = M_\tau u_n$$

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 $N_\tau$ 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 $\mathcal{V}_\tau$ 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 $\varepsilon$ versus the number of time steps $N_t$ for the soliton solutions of Eq. (7) with $\mathcal{O}(k) = k^2/2$.

The calculation results (points) are shown from top to bottom for $L_\tau$ (gray), $S_\tau$ (black), $B_\tau$ (brown), $Y_\tau$ (blue), $N_\tau$ (red), and $S_\tau$ (green). Straight lines correspond to the optimal fit $\varepsilon = C\tau^p$. For the first-order soliton in (a,b) we set $g = 1$, $X = 40$, $N_x = 2^9$ and either $T = 10$ (a) or $T = 40$ (b).

For the third-order soliton in (c,d) we set $g = 0.1$, $X = 200$, $N_x = 2^{10}$ and either $T = 20$ (c) or $T = 100$ (d).
**Figure**: Simulation errors $\varepsilon$ versus the number of time steps $N_t$ for the soliton solutions of Eq. (7) with $\mathcal{D}(k) = k^2/2$. 