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Preface

Splitting methods for differential equations

Splitting methods, associated with finite differences, finite elements, hybrid multi-scale settings or adaptations, have been widely used and shown to have powerful capabilities in solving all the major classes of different differential equations in various applications. Latest challenging research issues in the area range from splitting for higher accuracy and flexibility in different parallel environments, splitting for nonlinear partial differential equations, splitting for singular differential equations and inverse problems, nonlinear stability and convergence of splitting schemes, iterative and adaptive splitting strategies, geometric integration and domain decomposition methods, to quantum splitting computations in modern bio-chemistry and physics applications. Contributed from distinguished researchers in the aforementioned fields, this Special Issue is a first concentrated discussion that represents the exciting new era in the development of the splitting methods.

The original idea of the splitting methods can be traced back to 1898. Let $\mathcal{L}$ be a simply-connected Lie group with Lie algebra ℓ. If

$$\exp : \ell \longrightarrow \mathcal{L}$$

is the exponential map, then the solution of the equation

$$Z = \log(\exp(A)\exp(B)), \quad A,\ B \in \ell,$$

can be represented as a formal infinite sum of elements of ℓ, that is,

$$\begin{aligned}\log(\exp(A)\exp(B)) = A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] - \frac{1}{12}[B, [A, B]] \\ - \frac{1}{48}[B, [A, [A, B]]] - \frac{1}{48}[A, [B, [A, B]]] + \cdots ,\end{aligned}$$

where $[A, B]$ is the commutator of A and B. The above is often referred to as the *Baker-Campbell-Hausdorff formula.* It has been shown that there is no solution expression of Z in closed form for an arbitrary Lie algebra, except some exceptional tractable cases.

The Baker-Campbell-Hausdorff formula also has many important applications beyond mathematics, for instance, in quantum physics and astronomy. Interested readers are referred to publications by Chin, McLachlan, Suzuki and Yosida and references therein.

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Inspired by the Baker-Campbell-Hausdorff formula, modern splitting methods seek computationally applicable splitting approximations of the exponential function,

$$M(t) = \exp(tA), \quad t \geq t_0 > 0,$$

where A can be split additively into several pieces, that is,

$$A = \sum_{k=1}^{K} A_k$$

and $A_i, A_j, 1 \leq i, j \leq K$, do not, in general, commute. We are particularly interested in the approximant of the form,

$$S(t) = \sum_{m=1}^{M} \alpha_m \prod_{n=1}^{N(m)} \exp\left(\beta_{m,n} t A_{k(m,n)}\right),$$

where $\alpha_m,\ \beta_{m,n}$ are constants to be determined and $k(m,n) \in \{1, 2, \ldots, K\}$. We say that $S(t)$ is an *order ρ approximation of $M(t)$ with respect to t* if

$$\|S(t) - M(t)\| = O\left(t^{\rho+1}\right)$$

under a suitable norm $\|\cdot\|$. The function $S(t)$ is called an *exponential splitting,* or an *operator splitting,* of $M(t)$. Numerous important exponential splitting formulae have been developed and studied since the pioneer work of Douglas, Peaceman and Rachford on the ADI method in 1955. Denote $\exp(tC)$ as e^{tC}. Needless to say, the most popular splitting formulae in computational applications include the *first order splitting* S_1, *Strang's splitting* S_S, and the *parallel splitting* S_P :

$$\begin{aligned}
S_1(t) &= \mathrm{e}^{tA_1}\mathrm{e}^{tA_2}\cdots\mathrm{e}^{tA_{K-1}}\mathrm{e}^{tA_K},\\
S_\mathrm{S}(t) &= \mathrm{e}^{(t/2)A_1}\mathrm{e}^{(t/2)A_2}\cdots\mathrm{e}^{(t/2)A_{K-1}}\mathrm{e}^{tA_K}\mathrm{e}^{(t/2)A_{K-1}}\cdots\mathrm{e}^{(t/2)A_2}\mathrm{e}^{(t/2)A_1},\\
S_\mathrm{P}(t) &= \frac{1}{2}\left(\mathrm{e}^{tA_1}\mathrm{e}^{tA_2}\cdots\mathrm{e}^{tA_{K-1}}\mathrm{e}^{tA_K} + \mathrm{e}^{tA_K}\mathrm{e}^{tA_{K-1}}\cdots\mathrm{e}^{tA_2}\mathrm{e}^{tA_1}\right).
\end{aligned}$$

It is not difficult to verify that both S_S and S_P are of second order accuracy.

It may be interesting to mention that, under the positivity constraint required by the stability, that is, all coefficients $\alpha_m,\ \beta_{m,n}$ must be positive, the maximal order of an exponential splitting formula can only be two (Sheng [1] and Suzuki [2]).

We may acquire most of the known splitting schemes used today for solving differential equations by replacing the exponential functions in a splitting formula by appropriate rational approximations. For instance, the well-known two-dimensional Peaceman-Rachford algorithm in a continuing operation can be viewed as a combination of the second order [1/1] Padé approximant and the following slightly extended exponential splitting formula,

$$S_\text{P-R}(t) = \left(I - \frac{t}{2}B\right)^{-1} \mathrm{e}^{(t/2)A}\left(\mathrm{e}^{(t/2)A}\mathrm{e}^{tB}\mathrm{e}^{(t/2)A}\right)^{n-1}\mathrm{e}^{(t/2)A}\left(I + \frac{t}{2}B\right).$$

The above formula also reveals an embedded connection between the Peaceman-Rachford's ADI method and Strang's splitting, though the latter is far more general and important in the splitting theory and applications. Our readers are referred to Khaliq and Shengs' article in this Special Issue for details.

Based on the exciting results and discussions contained in this Special Issue, the readers are surely invited to explore and optimize different splitting schemes for their applications, beyond the traditional platform built by Douglas, Peaceman and Rachford, Marchuk and Samarskiǐ, Mitchell and Fairweather, D'Yakonov, Gordon and Gourlay, and Strang through combinations of novel exponential splitting formulae and rational approximations.

It has been evident that, as pointed out by authors of this Special Issue, splitting methods have been providing incredibly powerful and reliable computational tools for solving different partial differential equations. Splitting schemes are highly popular in real applications because of their outstanding simplicity in structures, great flexibility in working together with other numerical components, such as iteration and adaptation, and their exceptionally high efficiency in solution procedures. Many new concepts and splitting strategies have emerged, such as asymptotic splitting and hybrid splitting, in recent years.

The aim of this Special Issue is to highlight the new developments in the area within a limited content. The guest editors of this Special Issue would encourage the readers, while enjoying the remarkable results presented in this Special Issue, to participate in the many research activities in splitting theory and applications, and to continue to support and promote the study of splitting methods up to a new higher level in the near future.

Finally, the guest editors of this Special Issue would like to take this opportunity to thank Professor E. H. Twizell, Editor-in-Chief of *International Journal of Computer Mathematics,* for his wonderful foresight, encouragement, and guidance throughout the preparation of this Special Issue. The guest editors appreciate very much all the contributors and reviewers for their interest, hard work and commitment which have made this publication possible. The guest editors' sincere thanks also go to the team at Taylor & Francis; Lance Littlejohn, Frank Mathis and Robert Piziak of the Baylor University; Yuri Melnikov and Terrance Quinn of the Middle Tennessee State University; and Gilbert Strang of the Massachusetts Institute of Technology for their constant help and support during the editing work. The guest editors would like to thank again their wonderful colleagues, graduate students, NA-Digest and the Society for Industrial and Applied Mathematics (SIAM) for the many discussions and assistance received. Last, but not least, the guest editors wish to thank their families for the marvelous understanding and support during the many sleepless nights in fulfilling their research and editorial goals.

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