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High-order splitting methods for separable non-autonomous parabolic equations

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ABSTRACT

We consider the numerical integration of non-autonomous separable parabolic equations using high order splitting methods with complex coefficients (methods with real coefficients of order greater than two necessarily have negative coefficients). We propose to consider a class of methods that allows us to evaluate all time-dependent operators at real values of the time, leading to schemes which are stable and simple to implement. If the system can be considered as the perturbation of an exactly solvable problem and the flow of the dominant part is advanced using real coefficients, it is possible to build highly efficient methods for these problems. We show the performance of this class of methods on several numerical examples and present some new improved schemes.

1. Introduction

We consider the numerical integration of non-autonomous separable parabolic equations using high order splitting methods with complex coefficients. This class of methods has been recently used for the numerical integration of the autonomous case, showing good performances [5,11,16]. Splitting methods with real coefficients of order greater than two necessarily have negative coefficients and cannot be used for solving these problems [4,14,20,22]. However, solutions with complex coefficients with positive real part exist, and some of these methods can provide a high performance in spite of the fact that the equations have to be solved in the complex domain. Previous works with applications among others in celestial mechanics and quantum mechanics where splitting methods with complex coefficients are considered already exist [2,3,12,18,19,21–23].

A straightforward application of splitting methods with complex coefficients to non-autonomous problems requires the evaluation of the time-dependent functions on the operators at complex times, and the corresponding flows in the numerical scheme are, in general, not well conditioned. In this work we propose to consider a class of splitting methods in which one set of the coefficients belong to the class of real and positive numbers. This can allow to evaluate all time-dependent operators at real values of the time, leading to schemes which are stable and simple to implement.

If the system can be considered as the perturbation of an exactly solvable problem (or easy to numerically solve) and the flow of the dominant part is advanced using the real coefficients, it is possible to build highly efficient methods for these problems.

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1.1. The problem

Let us consider the non-autonomous separable PDE

$$\frac{du}{dt}=A(t,u)+B(t,u),\qquad u(0)=u_0, \tag{1.1}$$

$u(x,t)\in\mathbb{R}^D$, where the (possibly unbounded) operators A, B and $A+B$ generate C^0 semi-groups for positive t over a finite or infinite Banach space. Equations of this form are encountered in the context of *parabolic* partial differential equations, an example being the inhomogeneous non-autonomous *heat equation*

$$\frac{\partial u}{\partial t}=\alpha(t)\Delta u+V(x,t)u,\quad\text{or}\quad \frac{\partial u}{\partial t}=\nabla\big(a(x,t)\nabla u\big)+V(x,t)u \tag{1.2}$$

where $t\geq 0$, $x\in\mathbb{R}^d$ or $x\in\mathbb{T}^d$ and Δ denotes the Laplacian with respect to the spatial coordinates, x. Another example corresponds to reaction–diffusion equations of the form

$$\frac{\partial u}{\partial t}=D(t)\Delta u+B(t,u), \tag{1.3}$$

where $D(t)$ is a matrix of diffusion coefficients (typically a diagonal matrix) and B accounts for the reaction part. In general, $A(t,u)$, $B(t,u)$ can also depend on x, ∇, etc., which are omitted for clarity in the presentation.

For simplicity, we write the non-linear equation (1.1) in the (apparently) linear form

$$\frac{du}{dt}=L_{A(t,u)}u+L_{B(t,u)}u, \tag{1.4}$$

where L_A, L_B are the Lie operators associated with A, B, i.e.

$$L_{A(t,u)}\equiv A(t,u)\frac{\partial}{\partial u},\qquad L_{B(t,u)}\equiv B(t,u)\frac{\partial}{\partial u}$$

which act on functions of u.

If the problem is autonomous, the formal solution is given by $u(t)=\mathrm{e}^{t(L_{A(u)}+L_{B(u)})}u_0$, which is a short way to write

$$u(t)=\mathrm{e}^{t(L_{A(u)}+L_{B(u)})}u_0=\sum_{k=0}^{\infty}\frac{t^k}{k!}\left(A(u)\frac{\partial}{\partial u}+B(u)\frac{\partial}{\partial u}\right)^k u\,\bigg|_{u=u_0}.$$

If the subproblems

$$\frac{du}{dt}=A(u)\quad\text{and}\quad\frac{du}{dt}=B(u) \tag{1.5}$$

have exact solutions or can efficiently be numerically solved, it is usual to consider splitting methods as numerical integrators. If we denote by $\mathrm{e}^{hL_{A(u)}}$, $\mathrm{e}^{hL_{B(u)}}$ the exact h-flows for each problem in (1.5) (and for a sufficiently small time step, h) the simplest method within this class is the *Lie–Trotter splitting*

$$\mathrm{e}^{hL_{A(u)}}\mathrm{e}^{hL_{B(u)}}\quad\text{or}\quad\mathrm{e}^{hL_{B(u)}}\mathrm{e}^{hL_{A(u)}}, \tag{1.6}$$

which is a first order approximation in the time step to the solution, while the *symmetrized* version

$$S(h)=\mathrm{e}^{h/2L_{A(u)}}\mathrm{e}^{hL_{B(u)}}\mathrm{e}^{h/2L_{A(u)}}\quad\text{or}\quad S(h)=\mathrm{e}^{h/2L_{B(u)}}\mathrm{e}^{hL_{A(u)}}\mathrm{e}^{h/2L_{B(u)}} \tag{1.7}$$

is referred to as *Strang splitting*, and is an approximation of order 2, i.e. $S(h)=\mathrm{e}^{h(L_{A(u)+B(u)})}+\mathcal{O}(h^3)$. Upon using an appropriate sequence of steps, high-order approximations can be obtained as

$$\Psi(h)=\mathrm{e}^{hb_{m+1}L_B}\mathrm{e}^{ha_mL_A}\cdots\mathrm{e}^{hb_2L_B}\mathrm{e}^{ha_1L_A}\mathrm{e}^{hb_1L_B}, \tag{1.8}$$

and methods with real coefficients at any order can be obtained [13,21,25]. However, as already mentioned, splitting methods of order greater than two (with real coefficients) have at least one of the coefficients a_i negative as well as at least one of the coefficients b_i so, the flows e^{tL_A} and/or e^{tL_B} may not be well defined (this is indeed the case, for instance, for the Laplacian operator) and this prevents the use of methods which embed negative coefficients. For this reason, exponential splitting methods of at most order $p=2$ have been considered up to recently.

In order to circumvent this order-barrier, the papers [11] and [16] simultaneously presented a systematic analysis for a class of composition methods with complex coefficients having positive real parts. Using this extension from the real line to the complex plane, the authors of [11] and [16] built up methods of orders 3 to 14 by considering a technique known as *triple-jump composition*. More efficient high order methods are obtained in [5].