

Splitting Method of Convection-Diffusion Methods with Disentanglement methods

Disentanglement Methods

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Abstract In this paper, we discuss higher-order operator-splitting methods done by disentanglement methods. The idea is based on computing best fitted exponents to an exponential splitting scheme with more than two operators. We introduce the underlying splitting methods and the special scheme to compute the disentanglement method. First applications are done to consider finite difference methods to the spatial operators and derive their underlying Lie algebras. Based on the Lie algebra it is simple to compute the corresponding Lie group with exp functions. Such results help to derive the disentanglement of the operator splitting method. The verification of our improved splitting methods are done with first numerical examples.

Keywords. Operator splitting method, Iterative solver method, Distanglement method, Parabolic differential equations.

AMS subject classifications. 80A20, 80M25, 74S10, 76R50, 35J60, 35J65, 65M99, 65Z05, 65N12.

1 Introduction

Our motivation to study the splitting methods are coming from model equations which simulate bio-remediation [1] or radioactive contaminants [8], [7]. The efficiency of decoupling different physical processes, e.g. convection, reactions, help to accelerate the solver process, see [23].

In this paper we study the following model equations:

$$\partial_t c_i + \nabla \cdot (\mathbf{v}c_i - D\nabla c_i) = f_i(c_1, \dots, c_n), \text{ for } i = 1, \dots, n. \quad (1)$$

The unknown $c(x, t) = (c_1(x, t), \dots, c_n(x, t))^t$ is considered in $\Omega \times (0, T) \subset \mathbb{R}^d \times \mathbb{R}$, the space-dimension is given by d . The velocity \mathbf{v} is constant and D is the diffusion-dispersion tensor. The reaction $f_i(c_1, \dots, c_n)$ is a function of all unknowns c_i and couple the equations.

The aim of this paper is to study a novel splitting method which can improve standard operator splitting methods. First ideas are done with weighting methods which embed the so called is Zassenhaus product, see [24], we improve the initial and starting conditions of the splitting process. Here the ideas are to discuss the underlying Lie algebra, which are considered with the operators. Based on this information a more accurate approximation can be developed to derive the exponents of the splitting method.

The advantage is to apply standard spatial discretization methods to each operator and apply the resulting ordinary differential equation with the splitting method based on the disentanglement schemes.

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Further the novel method can be applied to iterative operator-splitting methods, which have some drawbacks in low convergence (see [28]), This can be improved by starting with sufficient accurate initial conditions, which is satisfied by weighting or disentanglement methods.

The outline of the paper is as follows. The operator-splitting-methods are introduced in the Section 2. Improvements of standard splitting methods to higher order splitting methods are discussed in Section 3. In Section ??, we discuss extension with to Zassenhaus product and the disentanglement methods. In Section 5, we present the numerical experiments and the benefits of the higher order splitting methods. Finally, we discuss future works in the area of iterative and non-iterative methods.

2 Operator splitting methods

We focus our attention on the case of two linear operators (i.e we consider the Cauchy problem):

$$\frac{\partial c(t)}{\partial t} = Ac(t) + Bc(t), \text{ with } t \in [0, T], c(0) = c_0, \quad (2)$$

whereby the initial function c_0 is given and A and B are assumed to be bounded linear operators in the Banach-space \mathbf{X} with $A, B : \mathbf{X} \rightarrow \mathbf{X}$. In realistic applications the operators corresponds to physical operators such as convection and diffusion operators. We consider the following operators splitting schemes:

1. Sequential operator-splitting: A-B splitting

$$\frac{\partial c^*(t)}{\partial t} = Ac^*(t) \text{ with } t \in [t^n, t^{n+1}] \quad \text{and} \quad c^*(t^n) = c_{sp}^n \quad (3)$$

$$\frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t) \quad \text{with } t \in [t^n, t^{n+1}] \quad \text{and} \quad c^{**}(t^n) = c^*(t^{n+1}), \quad (4)$$

for $n = 0, 1, \dots, N - 1$ whereby $c_{sp}^n = c_0$ is given from (2). The approximated split solution at the point $t = t^{n+1}$ is defined as $c_{sp}^{n+1} = c^{**}(t^{n+1})$.

2. Strang-Marchuk operator-splitting : A-B-A splitting

$$\frac{\partial c^*(t)}{\partial t} = Ac^*(t) \text{ with } t \in [t^n, t^{n+1/2}] \quad \text{and} \quad c^*(t^n) = c_{sp}^n \quad (5)$$

$$\frac{\partial c^{**}(t)}{\partial t} = Bc^{**}(t) \quad \text{with } t \in [t^n, t^{n+1/2}] \quad \text{and} \quad c^{**}(t^n) = c^*(t^{n+1/2}), \quad (6)$$

$$\frac{\partial c^{***}(t)}{\partial t} = Ac^*(t) \text{ with } t \in [t^{n+1/2}, t^{n+1}] \quad \text{and} \quad c^{***}(t^{n+1/2}) = c^{**}(t^{n+1/2}), \quad (7)$$

where $t^{n+1/2} = t^n + 0.5\tau_n$, and the approximated split solution at the point $t = t^{n+1}$ is defined as $c_{sp}^{n+1} = c^{***}(t^{n+1})$.

3. Iterative splitting with respect to one operator

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n, i = 1, 2, \dots, m \quad (8)$$

4. Iterative splitting with respect to alternating operators

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n \quad (9)$$

$$i = 1, 2, \dots, j,$$

$$\frac{\partial c_i(t)}{\partial t} = Ac_{i-1}(t) + Bc_i(t), \quad \text{with } c_{i+1}(t^n) = c^n, \quad (10)$$

$$i = j + 1, j + 2, \dots, m,$$

In addition, $c_0(t^n) = c^n$, $c_{-1} = 0$ and c^n is the known split approximation at the time level $t = t^n$. The split approximation at the time-level $t = t^{n+1}$ is defined as $c^{n+1} = c_{2m+1}(t^{n+1})$. (Clearly, the function $c_{i+1}(t)$ depends on the interval $[t^n, t^{n+1}]$, too, but, for the sake of simplicity, in our notation we omit the dependence on n .)

3 Zassenhaus Method and Disentanglement Method

Often standard splitting methods have the problem to be less effective in the rate of the convergence and CPU times.

To overcome this problem, we can enrich the approximation with higher order terms.

An improvement is done in the following way:

$$c_1(t) = \exp(At) \exp(Bt) \prod_{k=2}^i \exp(\hat{c}_k t^k) c_0, \quad (11)$$

where $c_i, i = 2, \dots, \infty$ are Zassenhaus exponents as follows:

$$\begin{aligned} c_2 &= -1/2[A, B], \\ c_3 &= (1/3[B, [B, A]] - 1/6[A, [A, B]]), \\ c_4 &= (-1/24[[[A, B], A], A] - 1/8[[[A, B], A], B] - 1/8[[[A, B], B], B]). \end{aligned} \quad (12)$$

Remark 1 The Zassenhaus method (see [25] and [16]) is derived as a composition of *exp*-functions and can be seen as an inverse to the BCH-Formula (Baker-Campbell-Hausdorff). Nevertheless, there exists not a closed derivation of the exponents. So numerical schemes are derived to compute the exponents in the Zassenhaus product.

Extended splitting method based on Zassenhaus-formula

In the next we enrich the standard splitting methods with the Zassenhaus method.

The standard exponential splitting methods are based on the following decomposition idea:

$$\exp((A + B)t) = \pi_{i=1}^j \exp(a_i At) \exp(b_i Bt) + O(t^{j+1}). \quad (13)$$

The extension to the exponential splitting schemes are given as:

$$\exp((A + B)t) = \pi_{i=1}^j \exp(a_i At) \exp(b_i Bt) \pi_{k=j}^m \exp(C_k t^k) + O(t^{m+1}). \quad (14)$$

where C_j is a function of Lie brackets of A and B .

Theorem 1 *The initial value problem (8) is solved by classical exponential splitting schemes. We assume bounded and constant operators A, B .*

Then we can find extensions based on the Zassenhaus formula given as

$$\exp((A + B)t) = \pi_{i=1}^j \exp(a_i At) \exp(b_i Bt) \pi_{k=j}^m \exp(C_k t^k) + O(t^{m+1}). \quad (15)$$

where C_j is a function of Lie brackets of A and B .

Proof 1.) Lie-Trotter splitting:

For the Lie-Trotter splitting there exists coefficients with respect to the extension:

$$\exp((A + B)t) = \exp(At) \exp(Bt) \prod_{k=2}^{\infty} \exp(C_k t^k), \quad (16)$$

where the coefficients C_k are given in [25].

Based on an existing BCH formula of the Lie-Trotter splitting one can apply the Zassenhaus formula.

2.) Strang Splitting:

A existing BCH formula is given as:

$$\exp(At/2) \exp(Bt) \exp(At/2) = \exp(tS_1 + t^3S_3 + t^5S_5 + \dots), \quad (17)$$

where the coefficients S_i are given as in [16].

There exists an Zassenhaus formula based on the BCH formula.

See:

$$\exp((A/2 + B/2)t) = \prod_{k=2}^{\infty} \exp(\tilde{C}_k t^k) \exp(A/2t) \exp(B/2t), \quad (18)$$

and

$$\exp((B/2 + A/2)t) = \exp(B/2t) \exp(A/2t) \prod_{k=2}^{\infty} \exp(C_k t^k), \quad (19)$$

then there exists a new product:

$$\prod_{k=3}^{\infty} \exp(D_k t^k) = \prod_{k=2}^{\infty} \exp(\tilde{C}_k t^k) \prod_{k=2}^{\infty} \exp(C_k t^k), \quad (20)$$

with one order higher, see also [32].

3.) General exponential splitting:

Same can be done with the general exponential splitting schemes.

Disentanglement of Exponential Operators

The disentanglement methods are used to approximate the exponential operators with respect to the underlying Lie algebra, see [26].

The disentangling problem is to solve the determination of the $\sigma_1, \dots, \sigma_m \in \mathbb{C}$ for a given Lie-Algebra $\{A_1, \dots, A_m\}$

The motivation is to find the smallest approximation, for example with 2 operators ($\{A, B\}$ are the generators of the finite dimensional Lie Algebra)

$$\exp(A + B) = \exp(\sigma_1 A_1) \dots \exp(\sigma_m A_m). \quad (21)$$

The idea is based on the Baker-Campbell-Hausdorff formula to extend the multiplication of $\exp(\sigma_1 A_1) \dots \exp(\sigma_m A_m)$ with the basis of the Lie-algebra generators: means:

$$\exp(\sigma_1 A_1) \dots \exp(\sigma_m A_m) \approx \exp(f_1^p(\sigma_1, \dots, \sigma_m) A_1 + \dots + f_m^p(\sigma_1, \dots, \sigma_m) A_m), \quad (22)$$

where $f_1^p, \dots, f_m^p : \mathbb{C}^m \rightarrow \mathbb{C}$ are functions developed on the order p of the BCH approximation.

Finally we have to solve a nonlinear equation system:

$$\begin{pmatrix} f_1^p(\tau_1, \dots, \tau_m) \\ \vdots \\ f_m^p(\tau_1, \dots, \tau_m) \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_m \end{pmatrix}, \text{ and } \sigma_k \approx \tau_k. \quad (23)$$

The computations can be done with Newton's iteration. To derive polynomials one have to apply algebraic coding e.g. in Mathematica see [26].

Simple Example: $\{A, B\}$ are generator of the Lie-Algebra $\{A, B\}$ where we assume $[A, B] = 0$. Then we can derive the BCH-Formula with respect to:

$$\exp(\sigma_1 A) \exp(\sigma_2 B) = \exp(\sigma_1 A + \sigma_2 B + \sigma_1 \sigma_2 [A, B] + \dots),$$

where $[A, B] = 0$ and all other commutators.

Therefore we have the know exact solution for a commutator group: $\sigma_1 = \sigma_2 = 1$.

We apply such methods for semi-discretized equation, especially Convection-Diffusion.

More applications are done in the following areas:

- Decoupling the equation to 2 or more operators, e.g. Kinetic and Potential operator, or Diffusion and Convection operator.
- Defining the Lie-algebra with the generators $\{A, B\}$
- Computing the disentanglement exponential operators on a sparse matrix structure and small matrix (less computational time).
- Computing with the disentanglement exponents, large sparse matrices.

Remark 2 The problem of the disentanglement methods are based on the underlying commutators, which have to be bounded in a numerical schemes, see [16]. If we consider bounded operators, we did not restrict the application of the method. By the way the more appropriate approximation is given to consider all commutators in the underlying algebra. Such schemes allows to minimize the computational time and obtain more accurate schemes.

4 Balancing of time and spatial discretization

Splitting methods are important for partial differential equations, because of reducing computational time to solve the equations and accelerating the solver process, see [12].

Here additional balancing is taken into account, because of the spatial step.

The following theorem, addresses the delicate situation of time and spatial steps and the fact of reducing the theoretical promised order of the scheme:

Theorem 2 We solve the initial value problem by applying iterative operator splitting schemes (9) and (10). We assume bounded and constant operators A, B . While iterating i -time with A and j -time with B the theoretical order is given as $O(t^{i+j})$. The initial step is given as $c_1(t) = \exp(At)\exp(Bt)c_0$.

Then we reduce order of the iterative scheme to $O(t^i)$, while norm of B is larger or equal than $O(\frac{1}{t})$ same is also with the operator A .

So the balancing below the so called CFL condition is important to preserve the order of the splitting method.

Proof The theoretical order of the iterative splitting scheme is given as:

$\|c_{i+j} - c\| \leq \|A\|\|B\|, t^{i+j} + O(t^{i+j+1})$ where $\|A\| = \rho(A)$ is the spectral or the maximum eigenvalue of operator A and $\|B\| = \rho(B)$ is the spectral or the maximum eigenvalue of operator B .

Based on the spatial discretization we have the following eigenvalues:

$\rho(A) = \frac{a_1}{\Delta x^p}, \rho(B) = \frac{a_2}{\Delta x^q}$ where we have a p -th order spatial discretization of A and a q -th order spatial discretization of B , a_1, a_2 are the diagonal entries of the finite difference stencil, see [13].

If we assume to have a CFL-condition ≥ 1 for the operator B we obtain:

$$\frac{a_1}{\Delta x^p} t \geq 1 \quad (24)$$

and therefore:

$$\|A_2\|^j t^j = O(1). \quad (25)$$

We lost the order for operator B and reduce to the order of the operator A .

Same can be done for operator A .

Therefore we have a necessary restriction to preserve the order of the splitting method given as:

$$O(1) \geq \rho(A) \geq O(\frac{1}{t}).$$

We preserve the order:

$$\|B\|^j t^j = O(t^j). \quad (26)$$

Remark 3 By using implicit method for the discretization scheme, we did not couple the time-scale and the spatial scale by a CFL condition and are so far independent of the reduction but taken into account less accurate results.

5 Numerical Examples

We consider the following test problems in order to verify our theoretical findings in the previous sections.

We discuss the application of the Zassenhaus product to iterative methods (e.g. iterative operator splitting methods) and non-iterative methods (e.g. Lie-Trotter, Strang splitting).

5.1 First Test- Example : Finite Difference Operators

We first deal with the following differential equation

$$\frac{\partial c(x, t)}{\partial t} = -\frac{\partial}{\partial x} c(x, t) + \frac{\partial^2}{\partial x^2} c(x, t), \quad (27)$$

$$c(x, t) = 0 \quad t \in [0, T], x = 0, x = L, \quad (28)$$

$$c(x, 0) = 1 \quad x \in [0, 1], \quad (29)$$

where $L = 10, T = 10$.

We apply finite difference and divide into 2 operators

$$A = \frac{1}{\Delta x} [-1 \ 1 \ 0]. \quad (30)$$

$$B = \frac{1}{\Delta x^2} [-1 \ 2 \ -1]. \quad (31)$$

We have the following Lie-Algebra:

$$I, A, B, [A, B], [A, [A, B]], [B, [B, A]]. \quad (32)$$

Our Lie group is given as:

$$\exp(I), \exp(A), \exp(B), \exp([A, B]), \exp([A, [A, B]]), \exp([B, [B, A]]). \quad (33)$$

Therefore the splitting method is given in the Zassenhaus formulation as:

$$\exp((A + B)t) = \exp(At) \exp(Bt) \exp(1/2[B, A]t^2) \exp((-1/6[A, [A, B]] + 1/3[B, [B, A]])t^3), \quad (34)$$

while the higher order terms are nearly zero and we can skip them.

See the computations of the operators:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}.$$

$$B = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}.$$

$$\exp((A + B)t) = \begin{pmatrix} 1.0305 & -0.0103 & 0.00005 \\ -0.0206 & 1.0306 & -0.0103 \\ 0.0002 & -0.0206 & 1.0305 \end{pmatrix}.$$

The commutators are given as: $f_1 = [B, A]$,

$$f_2 = [A, [A, B]],$$

$$f_3 = [B, [B, A]].$$

We compute the *exp*-functions:

$$Z_1 = \exp(At) \exp(Bt) = \begin{pmatrix} 1.03051 & -0.0103049 & 0.0000515236 \\ -0.0206099 & 1.03066 & -0.0103054 \\ 0.000206098 & -0.020611 & 1.03061 \end{pmatrix}.$$

$$Z_2 = \exp(At) \exp(Bt) \exp(1/2f_1t^2) = \begin{pmatrix} 1.03051 & -0.0103049 & 0.0000515233 \\ -0.0206101 & 1.03066 & -0.0103054 \\ 0.000206099 & -0.020611 & 1.0306 \end{pmatrix}.$$

$$Z_3 = \exp(At) \exp(Bt) \exp(1/2f_1t^2) \exp((-1/6f_2 + 1/3f_3)t^3) = \begin{pmatrix} 1.0305 & -0.0103 & 0.00005 \\ -0.0206 & 1.0306 & -0.0103 \\ 0.0002 & -0.0206 & 1.0305 \end{pmatrix}.$$

Numerical errors in the L_2 -norm are computed with time steps $t = 0.01$ in the next steps:

$$\|\exp((A + B)t) - Z_1\|_2 = 0.0000515287, \quad (35)$$

$$\|\exp((A + B)t) - Z_2\|_2 = 0.0000463758, \quad (36)$$

$$\|\exp((A + B)t) - Z_3\|_2 = 0.0000463752. \quad (37)$$

Z_i	L_2 error
Zassenhaus exponent	
Z_1	0.0000515287
Z_2	0.0000463758
Z_3	0.0000463752

For the disentanglement method we can achieve more accurate results.

The following Lie algebra $\{A, B, D, I, F\}$ is considered with the commutator relations:

$$[A, B] = -D, [B, D] = -I, [A, D] = -F, [A, I] = [B, I] = [D, I] = 0. \quad (38)$$

Our goal is to approximate the coefficients $\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5 \in \mathbb{C}$ such that

$$\exp((A + B)t) \approx \exp(\sigma_1 At) \exp(\sigma_2 Bt) \exp(\sigma_3 Dt^2) \exp(\sigma_4 It^3) \exp(\sigma_5 Ft^3), \quad (39)$$

where $D_5 = \exp(\sigma_1 A) \exp(\sigma_2 B) \exp(\sigma_3 D) \exp(\sigma_4 I) \exp(\sigma_5 F)$.

Some computations of the \exp -functions are given as:

$$\exp(A) = \begin{pmatrix} 7.38906 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -7.38906 & 7.38906 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3.69453 & -7.38906 & 7.38906 & 0 & 0 & 0 & 0 & 0 & 0 \\ -7.38906 & 0 & 0 & 7.38906 & 0 & 0 & 0 & 0 & 0 \\ 7.38906 & -7.38906 & 0 & -7.38906 & 7.38906 & 0 & 0 & 0 & 0 \\ -3.69453 & 7.38906 & -7.38906 & 3.69453 & -7.38906 & 7.38906 & 0 & 0 & 0 \\ 3.69453 & 0 & 0 & -7.38906 & 0 & 0 & 7.38906 & 0 & 0 \\ -3.69453 & 3.69453 & 0 & 7.38906 & -7.38906 & 0 & -7.38906 & 7.38906 & 0 \\ 1.84726 & -3.69453 & 3.69453 & -3.69453 & 7.38906 & -7.38906 & 3.69453 & -7.38906 & 7.38906 \end{pmatrix}.$$

$$\exp(B) = \begin{pmatrix} 137.872 & -118.716 & 51.1105 & -118.716 & 102.221 & -44.009 & 51.11050 & -44.009 & 18.94710 \\ -118.716 & 188.982 & -118.71 & 102.221 & -162.725 & 102.221 & -44.009 & 70.0576 & -44.009 \\ 51.1105 & -118.716 & 137.872 & -44.009 & 102.221 & -118.716 & 18.9471 & -44.009 & 51.1105 \\ -118.716 & 102.221 & -44.009 & 188.982 & -162.725 & 70.0576 & -118.716 & 102.221 & -44.009 \\ 102.221 & -162.725 & 102.221 & -162.725 & 259.04 & -162.725 & 102.221 & -162.725 & 102.22 \\ -44.009 & 102.221 & -118.716 & 70.0576 & -162.725 & 188.982 & -44.009 & 102.221 & -118.716 \\ 51.1105 & -44.009 & 18.9471 & -118.716 & 102.221 & -44.009 & 137.872 & -118.716 & 51.1105 \\ -44.009 & 70.0576 & -44.009 & 102.221 & -162.725 & 102.221 & -118.716 & 188.982 & -118.716 \\ 18.9471 & -44.009 & 51.1105 & -44.009 & 102.221 & -118.716 & 51.1105 & -118.716 & 137.872 \end{pmatrix}.$$

$$f_1 = [A, B],$$

$$\exp(f_1) = \begin{pmatrix} 0.13533 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.36787 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.36787 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.71828 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.71828 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.38906 \end{pmatrix},$$

$$f_2 = [A, [A, B]],$$

$$\exp(f_2) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 1 & 0.5 & 1 & 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0.25 & 0.5 & 0.5 & 0.5 & 1 & 1 & 0.5 & 1 & 1 \end{pmatrix}.$$

$$f_3 = [B, [B, A]],$$

$$\exp(f_3) = \begin{pmatrix} 0.3340 & 0.4036 & 0.2439 & 0.4036 & 0.4878 & 0.2947 & 0.2439 & 0.2947 & 0.1781 \\ -0.4036 & 0.0901 & 0.4036 & -0.4878 & 0.1089 & 0.4878 & -0.2947 & 0.0658 & 0.2947 \\ 0.2439 & -0.4036 & 0.3340 & 0.2947 & -0.4878 & 0.4036 & 0.1781 & -0.2947 & 0.2439 \\ -0.4036 & -0.4878 & -0.2947 & 0.0901 & 0.1089 & 0.0658 & 0.4036 & 0.4878 & 0.2947 \\ 0.4878 & -0.1089 & -0.4878 & -0.1089 & 0.0243 & 0.1089 & -0.4878 & 0.1089 & 0.4878 \\ -0.2947 & 0.4878 & -0.4036 & 0.0658 & -0.1089 & 0.0901 & 0.2947 & -0.4878 & 0.4036 \\ 0.2439 & 0.2947 & 0.1781 & -0.4036 & -0.4878 & -0.2947 & 0.3340 & 0.4036 & 0.2439 \\ -0.2947 & 0.06585 & 0.2947 & 0.4878 & -0.1089 & -0.4878 & -0.4036 & 0.0901 & 0.4036 \\ 0.1781 & -0.29475 & 0.2439 & -0.2947 & 0.4878 & -0.4036 & 0.24395 & -0.4036 & 0.3340 \end{pmatrix} \quad f_4 = [A, [A, [A, B]]],$$

$$\exp(f_4) = \begin{pmatrix} 0.1353 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.3678 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.3678 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2,7182 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2,7182 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.3890 \end{pmatrix}, \quad f_5 = [B, [B, [B, A]]],$$

$$\exp(f_5) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0.5 & 1 & 1 & 0.5 & 1 & 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0.25 & 0.5 & 0.5 & 0.5 & 1 & 1 & 0.5 & 1 & 1 \end{pmatrix},$$

We derive the exponents and achieve the same as for the Zassenhaus formula, given as:

$$Z_1 = \exp(At) \exp(Bt), \quad (52)$$

$$Z_2 = \exp(At) \exp(Bt) \exp(-1/2f_1), \quad (53)$$

$$Z_3 = \exp(At) \exp(Bt) \exp(-1/2f_1 t^2) \exp((-1/6f_2 + 1/3f_3)t^3), \quad (54)$$

where we apply $t = 0.01$.

The numerical errors with the L_2 norm are given as:

Z_i	L_2 error
Z_1	0.00010625
Z_2	0.000116874
Z_3	0.000116825

Remark 5 The same results can be obtained with larger matrices. Based on this results, the parameters can be computed with small matrices and less computational time.

6 Conclusion

In the paper we presented the benefits of improving standard splitting methods with Zassenhaus product and disentanglement methods. Such methods are extended splitting methods in weighting schemes. In first examples we could see benefits in more accuracy. By the way a next paper will discuss the convergence of such a scheme considering unbounded operators. Here we restrict us to bounded operators and nonstiff problems and discuss a novel method to derive exponential splitting schemes.

7 Appendix

Remark 6 To apply the exponential functions $\exp(At)$, etc. we apply the Pade approximations:

m / n	0	1	2	3
0	$\frac{1}{1}$	$\frac{1}{1-z}$	$\frac{1}{1-z+\frac{1}{2}z^2}$	$\frac{1}{1-z+\frac{1}{2}z^2-\frac{1}{6}z^3}$
1	$\frac{1+z}{1}$	$\frac{1+\frac{1}{2}z}{1-\frac{1}{2}z}$	$\frac{1+\frac{1}{3}z}{1-\frac{2}{3}z+\frac{1}{6}z^2}$	$\frac{1+\frac{1}{4}z}{1-\frac{3}{4}z+\frac{1}{4}z^2-\frac{1}{24}z^3}$
2	$\frac{1+z+\frac{1}{2}z^2}{1}$	$\frac{1+\frac{2}{3}z+\frac{1}{6}z^2}{1-\frac{1}{3}z}$	$\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	$\frac{1+\frac{2}{5}z+\frac{1}{20}z^2}{1-\frac{3}{5}z+\frac{3}{20}z^2-\frac{1}{60}z^3}$
3	$\frac{1+z+\frac{1}{2}z^2+\frac{1}{6}z^3}{1}$	$\frac{1+\frac{3}{4}z+\frac{1}{4}z^2+\frac{1}{24}z^3}{1-\frac{1}{4}z}$	$\frac{1+\frac{3}{5}z+\frac{3}{20}z^2+\frac{1}{60}z^3}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	$\frac{1+\frac{1}{2}z+\frac{1}{10}z^2+\frac{1}{120}z^3}{1-\frac{1}{2}z+\frac{1}{10}z^2-\frac{1}{120}z^3}$
4	$\frac{1+z+\frac{1}{2}z^2+\frac{1}{6}z^3+\frac{1}{24}z^4}{1}$	$\frac{1+\frac{4}{5}z+\frac{3}{10}z^2+\frac{1}{15}z^3+\frac{1}{120}z^4}{1-\frac{1}{5}z}$	$\frac{1+\frac{2}{3}z+\frac{1}{5}z^2+\frac{1}{30}z^3+\frac{1}{360}z^4}{1-\frac{1}{3}z+\frac{1}{30}z^2}$	$\frac{1+\frac{4}{7}z+\frac{1}{7}z^2+\frac{2}{105}z^3+\frac{1}{840}z^4}{1-\frac{3}{7}z+\frac{1}{14}z^2-\frac{1}{210}z^3}$

where we apply $m = n = 1$, $m = n = 2$ and $m = n = 3$.

Generalized Pade approximation

Remark 7 To apply the exponential functions $\exp(At)$, we apply the Pade approximations, that can be computed with a general scheme.

Here the idea of the Gauss continued fractions are considered, see [31]. The Pade approximants can be formulated in such a framework.

We define a first approximate ${}_1F_1(1; b; z)$ is given as

$${}_1F_1(1; b; z) = \frac{1}{1 + \frac{-z}{b + \frac{z}{(b+1) + \frac{-bz}{(b+2) + \frac{2z}{(b+3) + \frac{-(b+1)z}{(b+4) + \dots}}}}}, \quad (55)$$

and the application to $\exp(z) = {}_1F_1(1; 1; z)$

$$e^z = \frac{1}{1 + \frac{-z}{1 + \frac{z}{2 + \frac{-z}{3 + \frac{2z}{4 + \frac{-2z}{5 + \dots}}}}}}. \quad (56)$$

Then the Pade approximant is given as

$$R_{m,n} = \frac{{}_1F_1(-m; -m-n; z)}{{}_1F_1(-n; -m-n; -z)}, \quad (57)$$

where the standard notation for this series is given as

$${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z), \quad (58)$$

although variations are sometimes used see [30].

Using the rising factorial or Pochhammer symbol:

$$(a)_n = a(a+1)(a+2)\dots(a+n-1), \quad (a)_0 = 1, \quad (59)$$

this can be written

$${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z) = \sum_{n=0}^{\infty} \frac{(a_1)_n \dots (a_p)_n}{(b_1)_n \dots (b_q)_n} \frac{z^n}{n!}. \quad (60)$$

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