Iterative Operator Splitting Methods: Relation to Waveform Relaxation and Exponential Splitting Methods

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Abstract. In this paper we describe a technique for closed formulation of an iterative operator-splitting method and embed the method in the classical exponential splitting methods. Since iterative operator splitting have been developed, an abstract framework to relate the method to other classical splitting methods is needed. Here an abstract framework considering the iterative splitting method as waveform-relaxation or exponential splitting method is devised.

This is achieved by basing the analysis on semi-groups and fixed-point schemes.

Abstract results illustrate differential equations with constant and time-dependent coefficients.

Keywords Iterative operator-splitting method, Pade approximations.

AMS subject classifications. 65M15, 65L05, 65M71.

1 Introduction

In this paper we concentrate on approximation to the solution of the linear evolution equation

$$\partial_t u = Lu = (A+B)u, \ u(0) = u_0,$$
 (1)

where L, A and B are unbounded operators.

As numerical method we will employ a one-stage iterative splitting scheme, also known as the waveform-relaxation method:

$$u_i(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i-1} ds,$$
 (2)

where i = 1, 2, 3, ... and u0(t) = 0.

As a second numerical method we will employ a two-stage iterative splitting scheme :

$$u_i(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i-1} ds,$$
 (3)

$$u_{i+1}(t) = \exp(Bt)u_0 + \int_0^t \exp(Bs)Au_i \, ds,$$
 (4)

where $i = 1, 3, 5, \dots$ and u0(t) = 0.

The combination of both is given as an inner and outer iterative scheme:

$$u_{i_k}(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i_k+J_{k-1}-1} ds,$$
 (5)

$$u_{j_k+I_k}(t) = \exp(Bt)u_0 + \int_0^t \exp(Bs)Au_{j_k+I_k-1} ds,$$
 (6)

where $i_k = 1, 2, 3, ..., I_k$, $j_k = 1, 2, 3, ..., J_k$, k = 1, ..., K, $I_1, ..., I_K$ are the number of the iterations done with the A-operator, where $J_1, ..., J_K$ are are the number of iterations done with the B-operator. The initialization is given as u0(t) = 0 and $J_0 = 0$.

Here we combine the iterative steps for each operator, A and B.

The outline of the paper is as follows. The operator-splitting methods are introduced in Section 2. In Section 3, we discuss the error analysis of the different iterative methods and their benefits. In Section 4, we discuss an efficient computation of the iterative splitting method with a so-called closed formulation. In Section 5 we introduce the application of our methods to existing software tools. Finally, we discuss future works in the area of iterative methods.

2 Splitting method

Splitting methods are wel-known and often used to simplify and accelerate solver processes of differential equations, see [7], [9], [8], and [10].

While waveform-relaxation methods are studied extensively, see [17], [2], recently the iterative operator-splitting methods are studied as excellent decomposition methods to obtain higher-order results. First results are given in see [1], [3], [5], and [12].

Because of their structure a general splitting scheme can be derived, which is discussed in the following subsection.

2.1 Waveform relaxation method

The following algorithm is based on the iteration with fixed-splitting discretization step-size τ , namely, on the time-interval $[t^n, t^{n+1}]$ we solve the following sub-problems consecutively for $i = 1, 2, 3, \ldots, m$. (cf. [17]):

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n$$
 (7)

where c^n is the known split approximation at the time-level $t = t^n$, the initialization is $c_0(t) = c(t^n)$. The split approximation at the time-level $t = t^{n+1}$ is defined as $c^{n+1} = c_{m+1}(t^{n+1})$.

In the following we will analyze the convergence and the rate of convergence of the method (7) for m tends to infinity for the linear operators $A, B : \mathbf{X} \to \mathbf{X}$, where we assume that these operators and their sum are generators of the C_0 semi-groups. We emphasize that these operators are not necessarily bounded, so the convergence is examined in a general Banach space setting.

2.2Iterative splitting method

The following algorithm is based on the iteration with fixed-splitting discretization step-size τ , namely, on the time-interval $[t^n, t^{n+1}]$ we solve the following sub-problems consecutively for $i = 0, 2, \dots 2m$. (cf. [7, 12].):

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n
\text{and } c_0(t^n) = c^n, \ c_{-1} = 0.0,$$
(8)

and
$$c_0(t^n) = c^n$$
, $c_{-1} = 0.0$.

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

where 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.)

In the following we analyze the convergence and the rate of convergence of the method (8)–(9) for m tends to infinity for the linear operators $A, B: \mathbf{X} \to \mathbf{X}$, where we assume that these operators and their sum are generators of the C_0 semi-groups. We emphasize that these operators are not necessarily bounded, so the convergence is examined in a general Banach space setting.

General iterative splitting method

The combination of both methods means we are free to choose the number of iterative steps on each operator, and we obtain a scheme with inner and outer iterative schemes:

$$\frac{\partial c_{i_k+J_{k-1}}(t)}{\partial t} = Ac_{i_k+J_{k-1}}(t) + Bc_{i_k+J_{k-1}-1}(t), \text{ with } c_{i_k+J_{k-1}}(t^n) = c^n(10)$$

$$\frac{\partial c_{j_k+I_k}(t)}{\partial t} = Ac_{j_k+I_k-1}(t) + Bc_{j_k+I_k}(t), \text{ with } c_{j_k+I_k}(t^n) = c^n, \tag{11}$$

$$\frac{\partial c_{j_k + I_k}(t)}{\partial t} = Ac_{j_k + I_k - 1}(t) + Bc_{j_k + I_k}(t), \text{ with } c_{j_k + I_k}(t^n) = c^n,$$
 (11)

where $i_k = J_{k-1} + 1, \dots, I_k, j_k = I_k + 1, \dots, J_k, k = 1, \dots, K, I_k - J_{k-1}$ are the number of the iterations done with the A-operator, where $J_k - I_k$ are are the number of iterations done with the B-operator. The initialization is given as u0(t) = 0 and $I_0 = J_0 = 0$.

Here we combine the iterative steps for each operator, A and B.

3 Error analysis for the general scheme

In this section we analyze the convergence of the general scheme in which the waveform relaxation and iterative splitting method are embedded.

Theorem 1. Let us consider the abstract Cauchy problem in a Hilbert space X

$$\partial_t c(x,t) = Ac(x,t) + Bc(x,t), \quad 0 < t \le T \text{ and } x \in \Omega$$

$$c(x,0) = c_0(x) \ x \in \Omega$$

$$c(x,t) = c_1(x,t) \ x \in \partial\Omega \times [0,T],$$
(12)

where $A, B : D(\mathbf{X}) \to \mathbf{X}$ are given linear operators which are generators of the C_0 -semigroup and $c_0 \in \mathbf{X}$ is a given element. We assume A, B are unbounded. Further, we assume the estimations of the unbounded operator B with sufficient smooth initial conditions |9|:

$$||B \exp((A+B)\tau)u_0|| \le \kappa_1, \tag{13}$$

$$||A\exp((A+B)\tau)u_0|| \le \kappa_2,\tag{14}$$

Further, we assume the estimation with ϕ -functions:

$$||A\int_0^{\tau} \exp(As)u_0 ds|| \le \tau C_1 ||u_0||,$$
 (15)

$$||B\int_0^{\tau} \exp(Bs)u_0 ds|| \le \tau C_2 ||u_0||,$$
 (16)

The we can bound our iterative operator splitting method as:

$$||(S_i - \exp((A+B)\tau)u_0|| \le C\tau^i||u_0||, \tag{17}$$

where S_i is the approximated solution for the i-th iterative step and C is a constant that can be chosen uniformly on bounded time intervals.

Proof. Let us consider the iteration (10)–(11) on the sub-interval $[t^n, t^{n+1}]$. For the first iterations of (10) we have:

$$\partial_t c_1(t) = A c_1(t), \quad t \in (t^n, t^{n+1}],$$
 (18)

and for the second iteration we have:

$$\partial_t c_2(t) = Ac_2(t) + Bc_1(t), \quad t \in (t^n, t^{n+1}],$$
 (19)

In general, we have:

for m = 1, 2, ...,

$$\partial_t c_i(t) = Ac_i(t) + Bc_{i-1}(t), \quad t \in (t^n, t^{n+1}],$$
 (20)

where for $c_0(t) \equiv 0$.

We have the following solutions for the iterative scheme:

the solutions for the first two equations are given by the variation of constants:

$$c_1(t) = \exp(A(t^{n+1} - t))c(t^n), \quad t \in (t^n, t^{n+1}], \tag{21}$$

$$c_2(t) = \exp(At)c(t^n) + \int_{t^n}^{t^{n+1}} \exp(A(t^{n+1} - s))Bc_1(s)ds, \quad t \in (t^n, t^{n+1}], \quad (22)$$

for $m = 0, 1, 2, \dots$

$$c_i(t) = \exp(A(t - t^n))c(t^n) + \int_{t^n}^t \exp(sA)Bc_{i-1}(t^{n+1} - s) \ ds, \quad t \in (t^n, t^{n+1}],$$
(23)

The consistency is given as:

For e_1 we have:

$$c_1(\tau) = \exp(A)\tau)c(t^n),\tag{24}$$

$$c(\tau) = \exp((A+B)\tau)c(t^n) = \exp(A\tau)c(t^n)$$

$$+ \int_{t^n}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)(A+B))c(t^n) ds.$$
(25)

We obtain:

$$||e_1|| = ||c - c_1|| \le ||\exp((A + B)\tau)c(t^n) - \exp(A\tau)c(t^n)||$$
 (26)
 $\le C_1\tau||c(t^n)||.$

For e_2 we have:

$$c_{2}(\tau) = \exp(A\tau)c(t^{n}) + \int_{t^{n}}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)A)c(t^{n}) ds,$$
 (27)

$$c(\tau) = \exp(A\tau)c(t^{n}) + \int_{t^{n}}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)A)c(t^{n}) ds$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As)B$$

$$\int_{t^{n}}^{t^{n+1} - s} \exp(A\rho)B \exp((t^{n+1} - s - \rho)(A + B))c(t^{n}) d\rho ds.$$
(28)

We obtain:

$$||e_2|| \le ||\exp((A+B)\tau)c(t^n) - c_2||$$

 $\le C_2\tau^2||c(t^n)||.$ (29)

For the iterations, the recursive proof is given in the following:

for
$$m = 0, 1, 2, \ldots$$
, for e_i we have :

$$c_{i}(\tau) = \exp(A)\tau)c(t^{n})$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As)B \exp((t^{n+1} - s)A)c(t^{n}) ds$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1}$$

$$+ \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)uc(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - \sum_{j=1}^{i-1} s_{1}} \exp(s_{2}A)A \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - \sum_{j=1}^{i-1} s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - \sum_{j=1}^{i-1} s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1}} \exp(As_{1})B \int_{t^{n}}^{t^{n+1} - \sum_{j=1}^{i-1} s_{1}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})A)c(t^{n}) ds_{2} ds_{1} + \dots +$$

$$+ \int_{t^{n}}^{t^{n+1} - \sum_{j=1}^{i} s_{2}} \exp(s_{2}A)B \exp((\tau - s_{1} - s_{2})(A + B))c(t^{n}) ds_{i},$$

We obtain:

$$||e_i|| \le ||\exp((A+B)\tau)c(t^n) - c_i||$$

 $< C\tau^i||c(t^n)||,$ (32)

where $\alpha = \min_{i=1}^{i} {\{\alpha_1\}}$ and $0 \le \alpha_i < 1$.

The same proof idea can be applied to the other operator and we obtain:

Remark 1. The same idea can be applied with $A = \nabla D \nabla B = -\mathbf{v} \cdot \nabla$, so that one operator is less unbounded

but we reduce the convergence order

$$||e_1|| = K||B||\tau^{\alpha_1}||e_0|| + \mathcal{O}(\tau^{1+\alpha_1})$$
(33)

and hence

$$||e_2|| = K||B||||e_0||\tau^{1+\alpha_1+\alpha_2} + \mathcal{O}(\tau^{1+\alpha_1+\alpha}),$$
 (34)

where $0 \le \alpha_1, \alpha_2 < 1$.

Remark 2. If we assume the consistency of $\mathcal{O}(\tau^m)$ for the initial value $e_1(t^n)$ and $e_2(t^n)$, we can redo the proof and obtain at least a global error of the splitting methods of $\mathcal{O}(\tau^{m-1})$.

In the next section we describe the computation of the integral formulation with exp-functions.

4 Computation of the iterative splitting method: Closed formulation

In the last few years, computational attempts to compute integrals with expfunction have increased, and we present a closed form, and resubstitute the integral with closed functions. Such benefits accelerate the computation and parallel the ideas.

Here we present a closed form for the iterative splitting method for the first fourth splitting iterations:

For i = 1, we have

$$c_1(\tau) = \exp(A\tau) \exp(B\tau)c(t^n). \tag{35}$$

(36)

where we have a first-order method, also known as the AB splitting methods [1]. For i = 2, we have

$$c_2(\tau) = \frac{1}{2}(\exp(At)\exp(Bt) + \exp(Bt)\exp(At))$$
(37)

where we have a second order method, also known as the parallel AB splitting method [1].

For i = 3, we have:

$$c_3(\tau) = \frac{1}{6} (\exp(At) \exp(Bt) \exp(At) + \exp(Bt) \exp(At) \exp(At)$$
 (38)

$$+\exp(Bt)\exp(Bt)\exp(At) + \exp(At)\exp(At)\exp(Bt)$$
 (39)

$$+\exp(At)\exp(Bt)\exp(Bt) + \exp(Bt)\exp(At)\exp(Bt)) \tag{40}$$

where we can reduce the operators with assumptions to the commutators, e.g. [A, [A, B]] = [B, [A, A]].

Higher orders are at least the derivation of the remaining form of all the commutations.

4.1 Exp-Approximations with Pade approximations

In the applications, we have to extend differential equations to systems of differential equations. Therefore we have to apply matrix functions to our analytical tools.

To approximate matrix functions in the following section, we apply Pade approximations.

For the matrix exponential we apply:

$$\frac{I + \frac{1}{2}At}{I - \frac{1}{2}At} = \exp(At) + O((At)^3) , \qquad (41)$$

$$\frac{I + \frac{2}{3}(At) + \frac{1}{6}(At)^2}{I - \frac{1}{3}At} = \exp(At) + O((At)^4) , \qquad (42)$$

where $A \in \mathbb{R}^{n \times n}$ is the matrix and $I \in \mathbb{R}^{n \times n}$ is the identity matrix. We define the following matrix operator: $\frac{I}{L} = L^{-1}$ is the inverse matrix of $L \in \mathbb{R}^{n \times n}$, where L is non singular, see [15].

Remark 3. The general formulation for different Pade approximations to apply to exponential functions $\exp(At)$ is given in Table 1.

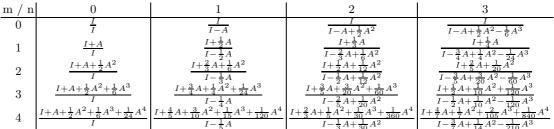


Table 1. Pade approximations of the exp-function.

In the next experiments, we apply the Pade approximations for m=n=1, m=n=2 and m=n=3.

5 Numerical experiments

5.1 First Experiment

We deal first with an ODE and separate the complex operator into two simpler operators.

We deal with the following equation :

$$\partial_t u_1 = -\lambda_1 u_1 + \lambda_2 u_2 \,, \tag{43}$$

$$\partial_t u_2 = \lambda_1 u_1 - \lambda_2 u_2 \,, \tag{44}$$

$$u_1(0) = u_{10} , u_2(0) = u_{20}$$
 (initial conditions) , (45)

where $\lambda_1, \lambda_2 \in \mathbb{R}^+$ are the decay factors and $u_{10}, u_{20} \in \mathbb{R}^+$. We have the time-interval $t \in [0, T]$.

We rewrite the equation (43) in operator notation, and we concentrate on the following equations:

$$\partial_t u = A(t)u + B(t)u , \qquad (46)$$

(47)

where $u_1(0) = u_{10} = 1.0$, $u_2(0) = u_{20} = 1.0$ are the initial conditions, where we have $\lambda_1(t) = t$ and $\lambda_2(t) = t^2$.

Our splitted operators are

$$A = \begin{pmatrix} -\lambda_1 \ \lambda_2 \\ 0 \ 0 \end{pmatrix} , B = \begin{pmatrix} 0 \ 0 \\ \lambda_1 - \lambda_2 \end{pmatrix} . \tag{48}$$

The concrete parameters for the experiments are given as:

 $\lambda_1 = 0.05 \ \lambda_2 = 0.01 \ T = 1.0 \ u_0 = (1, 1)^t$

We apply the AB, Stang and third order splitting and compare them with the unsplitted solutions:

(1.) Unsplitted:

$$c_{exact}(\tau) = \exp((A+B)\tau)c(t^n). \tag{49}$$

(2.) A-B splitting

$$c_1(\tau) = \exp(A\tau) \exp(B\tau)c(t^n). \tag{50}$$

where we have a first-order method, also known as the AB splitting methods [1].

(3.) Strang splitting

$$c_2(\tau) = \frac{1}{2}(\exp(At)\exp(Bt) + \exp(Bt)\exp(At))$$
(51)

where we have a second-order method, also known as parallel AB splitting method [1].

(4.) Third-order splitting

$$c_3(\tau) = \frac{1}{6} (\exp(At) \exp(Bt) \exp(At) + \exp(Bt) \exp(At) \exp(At) \exp(At) + \exp(Bt) \exp(Bt) \exp(At) + \exp(At) \exp(Bt) + \exp(At) \exp(Bt) + \exp(At) \exp(Bt) + \exp(Bt) \exp(Bt) + \exp(Bt) \exp(Bt)$$
(52)

where the solution is derived from the iterative splitting methods.

The L_1 -error is computed as:

$$err_{num} = \sum_{k=1}^{N} |u_{exact}(t_k) - u_{num}(t_k)|$$
 (53)

where $t_k = k\Delta t$, where t_0, t_1, \ldots and $\Delta t = 0.1$.

Remark 4. Our numerical results are based on higher order iterative schemes in closed formulations. Table 2 presents the results which show that third order methods can achieve more accurate results. The numerical results show that the splitting error decreases as long as the Pade approximation used allows it. Therefore we can say that more iterations are only sufficient when a method of higher order is used. One can also see that the iterative operator-splitting method is of order i as long as the Pade approximation is also of order i.

number of	err_1 (2nd order)	err_2 (2nd order)	err_1 (3rd order)	err_2 (3rd order)
time partitions				
2	4.5321e-002	3.6077e-003	4.5321e-002	3.6077e-003
3	4.6126e-004	3.6077e-003	4.6126e-004	3.6077e-003
4	4.6126e-004	2.2459e-005	4.6126e-004	2.2464e-005
5	1.9096e-006	2.2459e-005	1.9040e-006	2.2464e-005
6	1.9096e-006	6.1224e-008	1.9040e-006	6.6759 e - 008

Table 2. Numerical results for the first example with the iterative splitting method and second- and third-order method.

5.2 Second Experiment

We deal second with an ODE and separate the complex operator into two simpler operators.

We deal with the following equation:

$$\partial_t u_1 = -\lambda_1(t)u_1 + \lambda_2(t)u_2 , \qquad (54)$$

$$\partial_t u_2 = \lambda_1(t)u_1 - \lambda_2(t)u_2 , \qquad (55)$$

$$u_1(0) = u_{10} , u_2(0) = u_{20}$$
 (initial conditions) , (56)

where $\lambda_1(t) \in \mathbb{R}^+$ and $\lambda_2(t) \in \mathbb{R}^+$ are the decay factors and $u_{10}, u_{20} \in \mathbb{R}^+$. We have the time-interval $t \in [0, T]$.

We rewrite the equation (54) in operator notation, and we concentrate on the following equations:

$$\partial_t u = A(t)u + B(t)u , \qquad (57)$$

(58)

where $u_1(0) = u_{10} = 1.0$, $u_2(0) = u_{20} = 1.0$ are the initial conditions, where we have $\lambda_1(t) = t$ and $\lambda_2(t) = t^2$.

Our splitted operators are

$$At = \begin{pmatrix} -\lambda_1(t) \ \lambda_2(t) \\ 0 \ 0 \end{pmatrix}, Bt = \begin{pmatrix} 0 & 0 \\ \lambda_1(t) - \lambda_2(t) \end{pmatrix}.$$
 (59)

For the equation (54), we could apply a higher-order Pade approximation, e.g. third order.

We apply first the sequential splitting and the iterative operator-splitting, and then we combine them by using the pre-step based methods to see the improved results.

For the time-steps Δt we have $\Delta t=1$ for 1 time-partition and $\Delta t=0.1$ for 10 time-partitions.

Remark 5. Our numerical results are based on higher order iterative schemes in closed formulations. Table 3 presents the results which show that third order methods can achieve more accurate results. By the way the more time-dependent

number of	err_1 (2nd order)	err_2 (2nd order)	err_1 (3rd order)	err_2 (3rd order)
time partitions				
1	4.5541e-001	3.6275e-002	4.6325e-001	3.8057e-002
10	4.5146e-004	3.7277e-003	4.4136e-004	3.8277e-003

Table 3. Numerical results for the second example with the iterative splitting method and second- and third-order method.

operators need more time partitions to obtain the same accurate results as with constant operators. Here numerical results show that the splitting error decreases as long as the balance between number of time partitions and higher order approximations are used. The Pade approximation has to be of order i as long as the iterative scheme has also the order i.

6 Conclusions and Discussions

We have presented an iterative operator-splitting method and analyze the error bound for unbounded operators. Under weak assumptions we could prove the higher-order error bounds. Numerical examples confirm the applications to differential equations. In the future we will focus on the development of improved operator-splitting methods with respect to their application in nonlinear differential equations.

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