Nonlinear Iterative Operator-Splitting Methods and Applications for Nonlinear Parabolic Partial Differential Equations

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Abstract. In this paper we concentrate on nonlinear iterative operator splitting methods for nonlinear differential equations. The motivation arose from decoupling nonlinear operator equations in simpler operator equations. The decomposition in simpler equations allow to apply adaptive time-discretization methods in each underlying time-scale. Therefore one can solve the equations more effectively and accurate. The underlying coupling of the splitting method is fulfilled with a relaxation, coming from the results of the previous time-steps, the adapted problems. We consider the consistency and stability analysis of the nonlinear iterative operator splitting method. The consistency analysis is based on linearization. An a priori error estimates is derived for the linearized case. Finally we discuss the iterative operator-splitting methods for the applications to multi-physics problems.

Keywords. Operator Splitting method, Iterative Solver methods, relaxation methods, consistency analysis, stability analysis, multi-physics problems.

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1 Introduction

Our motivation came from designing effective algorithms for large equation systems. The problem arose in the field of scientific computing of very large systems of partial differential equations fixed on time-scale and on one discretization method. Effective computational methods can derived by considering the local character of each equation part. So in the last years the ideas of splitting into simpler equations are established, see [18], [24] and [17]. We concentrate on robust methods based on the relaxation theory to decouple in a system of simpler equations and solve each part with the locally adapted discretization and solver methods, see cite. A nonlinear operator-splitting method is presented and explained in the context of the consistency of a linearized method. For a stable method we modify our method to a weighted iterative splitting method and can derive a strong stability result. The a priori error-estimates and the decomposition characteristic is discussed. Applications in multi physics problems based on linear and nonlinear differential equations are considered.

The paper is organized as follows. A mathematical model based on the convection-reaction equations is introduced in section 2. The consistency of the linear and nonlinear iterative operator-splitting methods are described in section 3. In section 4 we introduce the stability analysis of the methods and derive the strong stability. The a posteriori error estimates is discussed in section 5 and the discretization methods are described in section 6. We introduce the numerical results in section 7. Finally we discuss our future works in the area of splitting and decomposition methods.

2 Mathematical Model

Our model equations are coming from a computational simulation of bio-remediation [3] or radioactive contaminants [10], [9].

The mathematical equations are system of parabolic partial differential equations given by

$$\partial_t C + V\nabla C - \nabla \cdot D\nabla C = F(C) , \text{ in } \Omega \times [0, T] , \qquad (1)$$

$$C(x,0) = C_0(x) , \text{ in } \Omega , \qquad (2)$$

$$C(x,t) = (0,\ldots,0)^t, \text{ on } \partial \Omega \times [0,T].$$
(3)

The unknown $C = C(x,t) = (c_1(x,t), \ldots, c_n(x,t))^T$ are considered in $\Omega \times (0,T) \subset \mathbb{R}^d \times \mathbb{R}$, the space-dimension is given by d and n is the number of equations. The convective part is given as $V\nabla C = (v_1\nabla c_1, \ldots, v_n\nabla c_n)^t$, where $v_1, \ldots, v_n \in \mathbb{R}^+$ are the constant vectorial velocities. Further the diffusion part is given as $\nabla \cdot D\nabla C = (D_1\nabla c_1, \ldots, D_n\nabla c_n)^t$, where $D_1, \ldots, D_n \in \mathbb{R}^+$ are the constant scalar diffusion-parameters. Our reaction part is given as $F(C) = f_1(c_1, \ldots, c_n), \ldots, f_n(c_1, \ldots, c_n)$, with the nonlinear functions $f_1, \ldots, f_n : \mathbb{R}^n \to \mathbb{R}$.

The aim of this paper is to present nonlinear and stable iterative operatorsplitting methods for nonlinear differential equations.

3 Consistency Theory for the linear and nonlinear iterative splitting method

3.1 Linear iterative splitting method

The following algorithm is based on the iteration with fixed splitting discretization step-size τ . On the time interval $[t^n, t^{n+1}]$ we solve the following subproblems consecutively for $i = 1, 3, \ldots, 2m + 1$. (cf. [18] and [8].)

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n , \qquad (4)$$

$$\frac{\partial c_{i+1}(t)}{\partial t} = Ac_i(t) + Bc_{i+1}(t), \text{ with } c_{i+1}(t^n) = c^n , \qquad (5)$$

 $\mathbf{2}$

where $c_0 \equiv 0$ 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.)

In the following we will analyze the convergence and the rate of the convergence of the method (4)–(5) 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 semigroup. We emphasize that these operators aren't necessarily bounded, so, the convergence is examined in general Banach space setting.

Theorem 1. Let us consider the abstract Cauchy problem in a Banach space \mathbf{X}

$$\partial_t c(t) = Ac(t) + Bc(t), \quad 0 < t \le T ,$$

$$c(0) = c_0 .$$
(6)

where $A, B, A + B : \mathbf{X} \to \mathbf{X}$ are given linear operators being generators of the C_0 -semigroup and $c_0 \in \mathbf{X}$ is a given element. Then the iteration process (4)–(5) is convergent and the rate of the convergence is of higher order.

The proof could be found in [8].

The a priori error-estimates is given in the following theorem.

Theorem 2. The estimate (30) shows that after iteration step (i = 2m + 1) we have the estimation

$$\|e_{2m+1}\| = K_m \|e_0\| \tau_n^{2m} + \mathcal{O}(\tau_n^{2m+1}).$$
(7)

where $c_0(t)$ is the initial guess, see [18].

Remark 1. When A and B are matrices (i.e. (4)-(5) is a system of ordinary differential equations), for the growth estimation we can use the concept of the logarithmic norm. (See e.g.[17].) Hence, for many important classes of matrices we can prove the validity.

Remark 2. We note that a huge class of important differential operators generate contractive semigroup. This means that for such problems -assuming the exact solvability of the split sub-problems- the iterative splitting method is convergent in higher order to the exact solution.

3.2 Consistency nonlinear iterative splitting method

Theorem 3. Let us consider the nonlinear operator-equation in a Banach space \mathbf{X}

$$\partial_t c(t) = A(c(t)) + B(c(t)), \quad 0 < t \le T,$$

 $c(0) = c_0,$
(8)

We linearized the nonlinear operators and obtain the linearized equation

$$\partial_{t}c(t) = \tilde{A}c(t) + \tilde{B}c(t) + R(\tilde{c}), \quad 0 < t \leq T ,$$

$$\tilde{A} = \frac{\partial A}{\partial c}(\tilde{c}) ,$$

$$\tilde{B} = \frac{\partial B}{\partial c}(\tilde{c}) ,$$

$$R(\tilde{c}) = A(\tilde{c}) + B(\tilde{c}) - \tilde{c}(\frac{\partial A}{\partial c}(\tilde{c}) + \frac{\partial B}{\partial c}(\tilde{c})) ,$$

$$c(0) = c_{0} ,$$

(9)

where $\tilde{A}, \tilde{B}, A + B : \mathbf{X} \to \mathbf{X}$ are given linear operators being generators of the C_0 -semigroup and $c_0 \in \mathbf{X}$ is a given element. Then the iteration process (4)–(5) is convergent and the rate of the convergence is of second order.

We obtain the iterative result :

Proof. Let us consider the iteration (4)–(5) on the sub-interval $[t^n, t^{n+1}]$. For the error function $e_i(t) = c(t) - c_i(t)$ we have the relations

$$\partial_t e_i(t) = A(e_i(t)) + B(e_{i-1}(t)), \quad t \in (t^n, t^{n+1}], \\ e_i(t^n) = 0,$$
(10)

and

$$\partial_t e_{i+1}(t) = A(e_i(t)) + B(e_{i+1}(t)), \quad t \in (t^n, t^{n+1}], \\ e_{i+1}(t^n) = 0,$$
(11)

for $m = 0, 2, 4, \ldots$, with $e_0(0) = 0$ and $e_{-1}(t) = c(t)$.

In the following we derive the linearized equations. We use the notations \mathbf{X}^2 for the product space $\mathbf{X} \times \mathbf{X}$ enabled with the norm $||(u, v)|| = \max\{||u||, ||v||\}$ $(u, v \in \mathbf{X})$. The elements $\mathcal{E}_i(t), \mathcal{F}_i(t) \in \mathbf{X}^2$ and the linear operator $\mathcal{A} : \mathbf{X}^2 \to \mathbf{X}^2$ are defined as follows

$$\mathcal{E}_{i}(t) = \begin{bmatrix} e_{i}(t) \\ e_{i+1}(t) \end{bmatrix}; \quad \mathcal{A} = \begin{bmatrix} \frac{\partial A(c_{i-1})}{\partial c} & 0 \\ \frac{\partial A(c_{i-1})}{\partial c} & \frac{\partial B(c_{i-1})}{\partial c} \end{bmatrix}, \quad (12)$$

$$\mathcal{F}_{i}(t) = \begin{bmatrix} A(e_{i-1}(t)) + B(e_{i-1}(t)) - e_{i-1} \frac{\partial A(e_{i-1})}{\partial c} \\ A(e_{i-1}(t)) + B(e_{i-1}(t)) - e_{i-1} \frac{\partial A(e_{i-1})}{\partial c} - e_{i-1} \frac{\partial B(e_{i-1})}{\partial c} \end{bmatrix} .$$
(13)

Then, using the notations (13), the relations (10)-(11) can be written in the form

$$\partial_t \mathcal{E}_i(t) = \mathcal{A} \mathcal{E}_i(t) + \mathcal{F}_i(t), \quad t \in (t^n, t^{n+1}],$$

$$\mathcal{E}_i(t^n) = 0.$$
 (14)

Due to our assumptions, \mathcal{A} is a generator of the one-parameter C_0 semigroup $(\mathcal{A}(t))_{t\geq 0}$. We also assume the estimation of our term $\mathcal{F}_i(t)$ with the growth conditions.

Remark 3. We can estimate the nonlinear operators $A(e_{i-1})$ and $B(e_{i-1})$ by assuming the constant derivation $\frac{\partial A}{\partial c}$ and $\frac{\partial B}{\partial c}$ by the following equation :

$$||A(e_{i-1})|| = ||\int_0^1 \frac{\partial A}{\partial c}(c(t) + \theta e_{i-1}) e_{i-1} d\theta|| \le C||e_{i-1}||, \qquad (15)$$

where $e_{i-1}(t) = c(t) - c_{i-1}(t)$ and $|| \cdot ||$ is the maximum norm over t. The same we could use for the operator $B(e_{i-1})$.

We could estimate the right hand side $\mathcal{F}_i(t)$ in the following lemma :

Lemma 1. Let us consider the the bounded Jacobian of A(u) and B(u)We could then estimate the $\mathcal{F}_i(t)$ as

$$||\mathcal{F}_{i}(t)|| \le C||e_{i-1}||$$
 (16)

Proof. We have the following norm $||\mathcal{F}_i(t)|| = \max\{\mathcal{F}_{i_1}(t), \mathcal{F}_{i_1}(t)\}.$ We have to estimate each term :

$$\begin{aligned} ||\mathcal{F}_{i_{1}}(t)|| &\leq ||A(e_{i-1}(t)) + B(e_{i-1}(t)) - e_{i-1}\frac{\partial A(e_{i-1})}{\partial c}|| \\ &\leq C_{1}||e_{i-1}(t)|| , \\ ||\mathcal{F}_{i_{2}}(t)|| &\leq ||A(e_{i-1}(t)) + B(e_{i-1}(t)) - e_{i-1}\frac{\partial A(e_{i-1})}{\partial c} - e_{i-1}\frac{\partial B(e_{i-1})}{\partial c} \\ &\leq C_{2}||e_{i-1}(t)|| . \end{aligned}$$
(17)

So we obtain the estimation : \tilde{r}

$$||\mathcal{F}_i(t)|| \le C||e_{i-1}(t)||$$

where \tilde{C} is the maximum value of C_1 and C_2 .

Hence using the variations of constants formula, the solution of the abstract Cauchy problem (14) with homogeneous initial condition can be written as

$$\mathcal{E}_i(t) = \int_{t^n}^t \exp(\mathcal{A}(t-s))\mathcal{F}_i(s)ds, \quad t \in [t^n, t^{n+1}].$$
(19)

(See, e.g. [6].) Hence, using the denotation

$$\|\mathcal{E}_{i}\|_{\infty} = \sup_{t \in [t^{n}, t^{n+1}]} \|\mathcal{E}_{i}(t)\| , \qquad (20)$$

we have

$$\|\mathcal{E}_{i}\|(t) \leq \|\mathcal{F}_{i}\|_{\infty} \int_{t^{n}}^{t} \|\exp(\mathcal{A}(t-s))\| ds =$$

$$= C \|e_{i-1}\| \int_{t^{n}}^{t} \|\exp(\mathcal{A}(t-s))\| ds, \quad t \in [t^{n}, t^{n+1}].$$
(21)

We have estimate $||\mathcal{F}_i|| \leq C ||e_{i-1}||$, where C is a constant that bounds the nonlinear terms of $\mathcal{F}_i(t)$.

Since $(\mathcal{A}(t))_{t\geq 0}$ is a semigroup therefore the so called *growth estimation*

$$\|\exp(\mathcal{A}t)\| \le K \exp(\omega t); \quad t \ge 0 , \qquad (22)$$

holds with some numbers $K \ge 0$ and $\omega \in \mathbb{R}$, see [6].

- Assume that $(\mathcal{A}(t))_{t\geq 0}$ is a bounded or exponentially stable semigroup, i.e. (22) holds with some $\omega \leq 0$. Then obviously the estimate

$$\|\exp(\mathcal{A}t)\| \le K; \quad t \ge 0, \qquad (23)$$

holds, and, hence on base of (10), we have the relation

$$\|\mathcal{E}_i\|(t) \le K\tau_n \|e_{i-1}\|, \quad t \in (0, \tau_n).$$
(24)

- Assume that $(\mathcal{A}(t))_{t\geq 0}$ has an exponential growth with some $\omega > 0$. Using (10) we have

$$\int_{t^n}^{t^{n+1}} \|\exp(\mathcal{A}(t-s))\| ds \le K_{\omega}(t), \quad t \in [t^n, t^{n+1}],$$
(25)

where

$$K_{\omega}(t) = \frac{K}{\omega} \left(\exp(\omega(t - t^{n})) - 1 \right), \quad t \in [t^{n}, t^{n+1}],$$
(26)

and hence

$$K_{\omega}(t) \le \frac{K}{\omega} \left(\exp(\omega \tau_n) - 1 \right) = K \tau_n + \mathcal{O}(\tau_n^2) , \qquad (27)$$

so the estimations (24) and (27) result in

$$\|\mathcal{E}_{i}\|_{\infty} = K\tau_{n} \|e_{i-1}\| + \mathcal{O}(\tau_{n}^{2}).$$
(28)

Taking into the account the definition of \mathcal{E}_i and the norm $\|\cdot\|_{\infty}$, we obtain

$$||e_i|| = K\tau_n ||e_{i-1}|| + \mathcal{O}(\tau_n^2),$$
(29)

and hence

$$||e_{i+1}|| = K_1 \tau_n^2 ||e_{i-1}|| + \mathcal{O}(\tau_n^3),$$
(30)

which proves our statement.

4 Stability Theory

We concentrate on the stability theory for the linear ordinary differential equations with commutative operators. First we apply the recursion for the general case and obtain the commutative case.

In the following we propose the weighted methods.

4.1 Weighted Iterative Splitting Method

The proposed un-symmetric weighted iterative splitting method is a combination between the sequential splitting method, see [7], and the iterative operator splitting method, see [8]. The weighting factor ω is used as an adaptive switch between lower and higher order splitting methods. The following algorithm is based on the iteration with fixed splitting discretization step-size τ . On the time interval $[t^n, t^{n+1}]$ we solve the following sub-problems consecutively for $i = 0, 2, \ldots 2m$.

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + \omega Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n \tag{31}$$

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

$$\frac{\partial c_{i+1}(t)}{\partial t} = \omega \ Ac_i(t) + Bc_{i+1}(t), \tag{32}$$

with $c_{i+1}(t^n) = \omega \ c^n + (1-\omega) \ c_i(t^{n+1})$,

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 $c^{n+1} = c_{2m+1}(t^{n+1})$. Our parameter $\omega \in [0, 1]$. For $\omega = 0$ we have the sequential-splitting and for $\omega = 1$ we have the iterative splitting method, cf. [8].

Because of the weighting between the sequential splitting and iterative splitting method, also the initial-conditions are weighted. So, we have the final results of the first equation (31) appearing in the initial condition for the second (32).

4.2 Damped Iterative Splitting Method

A next stable version is the damped iterative splitting method. In this version we concentrate on the examples with very stiff operators, e.g. *B*-operator. For initial solutions far away form the local solution, we have strong oscillations, see [16], [14]. Therefore we damp the *B*-operator in the case, that we relax in the initial steps with factors $\omega \approx 0$.

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

$$\frac{\partial c_i(t)}{\partial t} = Ac_i(t) + 2(1-\omega) Bc_{i-1}(t), \text{ with } c_i(t^n) = c^n$$
(33)
and $c_i(t^n) = c^n - c_{i-1} = 0.0$

and
$$c_0(t^{-}) = t^{-}$$
, $c_{-1} = 0.0$,
 $\frac{\partial c_{i+1}(t)}{\partial t} = \omega A c_i(t) + 2\omega B c_{i+1}(t)$, (34)
with $c_{i+1}(t^n) = c^n$,

where c^n is the known split approximation at the time level $t = t^n$. Our parameter $\omega \in [0, 1/2]$. For $\omega = 0$ we have the full damped method, and solving only operator A and for $\omega = 1/2$ we have the iterative splitting method, cf. [8].

Because of the weighting between the sequential splitting and iterative splitting method, also the initial-conditions are weighted. So, we have the final results of the first equation (33) appearing in the initial condition for the second (34).

4.3 Recursion for the stability results

First we concentrate on the weighted iterative splitting method, (31) and (32). We treat the special case for the initial-values with $c_i(t^n) = c_n$ and $c_{i+1}(t^n) = c_n$ for an overview. The general case $c_{i+1}(t^n) = \omega c_n + (1 - \omega)c_i(t^{n+1})$ could be treated in the same manner.

We consider the suitable vector norm $|| \cdot ||$ on \mathbb{R}^M , together with its induced operator norm. The matrix exponential of $Z \in \mathbb{R}^{M \times M}$ is denoted by $\exp(Z)$. We assume that

$$||\exp(\tau A)|| \le 1$$
 and $||\exp(\tau B)|| \le 1$ for all $\tau > 0$

It can be shown that the system (31)–(32) implies $||\exp(\tau (A+B))|| \le 1$ and is itself stable.

For the linear problem (31)-(32) it follows by integration that

$$c_i(t) = \exp((t-t^n)A)c^n + \int_{t^n}^t \exp((t-s)A) \ \omega \ Bc_{i-1}(s) \ ds \ , \tag{35}$$

$$c_{i+1}(t) = \exp((t-t^n)B)c^n + \int_{t^n}^t \exp((t-s)B) \ \omega \ Ac_i(s) \ ds \ . \tag{36}$$

With elimination of c_i we get

$$c_{i+1}(t) = \exp((t-t^n)B)c^n + \omega \int_{t^n}^t \exp((t-s)B) A \exp((s-t^n)A) c^n ds + \omega^2 \int_{s=t^n}^t \int_{s'=t^n}^s \exp((t-s)B) A \exp((s-s')A) B c_{i-1}(s') ds' ds .$$
 (37)

For the following commuting case we could evaluate the double integral $\int_{s=t^n}^t \int_{s'=t^n}^s \text{ as } \int_{s'=t^n}^t \int_{s=s'}^t$ and could derive the weighted stability-theory.

4.4 Commuting operators

For more transparency of the formula (37) we consider a well-conditioned system of eigenvectors and the eigenvalues λ_1 of A and λ_2 of B instead of the operators A, B themselves. Replacing the operators A and B by λ_1 and λ_2 respectively, we obtain after some calculations

$$c_{i+1}(t) = c^n \frac{1}{\lambda_1 - \lambda_2} \left(\omega \lambda_1 \exp((t - t^n) \lambda_1) + ((1 - \omega) \lambda_1 - \lambda_2) \exp((t - t^n) \lambda_2) \right) + c^n \omega^2 \frac{\lambda_1 \lambda_2}{\lambda_1 - \lambda_2} \int_{s=t^n}^t \left(\exp((t - s) \lambda_1) - \exp((t - s) \lambda_2) \right) ds .$$
(38)

Note that this relation is symmetric in λ_1 and λ_2 .

Strong Stability We define $z_k = \tau \lambda_k$, k = 1, 2. We start with $c_0(t) = c^n$ and we obtain

$$c_{2m}(t^{n+1}) = S_m(z_1, z_2) \ c^n , \qquad (39)$$

where S_m is the stability function of the scheme with *m*-iterations. We use (38) and obtain after some calculations

$$S_{1}(z_{1}, z_{2}) = \omega^{2} c^{n} + \frac{\omega z_{1} + \omega^{2} z_{2}}{z_{1} - z_{2}} \exp(z_{1}) c^{n}$$

$$+ \frac{(1 - \omega - \omega^{2}) z_{1} - z_{2}}{z_{1} - z_{2}} \exp(z_{2}) c^{n} ,$$
(40)

$$S_{2}(z_{1}, z_{2}) = \omega^{4} c^{n} + \frac{\omega z_{1} + \omega^{4} z_{2}}{z_{1} - z_{2}} \exp(z_{1}) c^{n}$$

$$+ \frac{(1 - \omega - \omega^{4}) z_{1} - z_{2}}{z_{1} - z_{2}} \exp(z_{2}) c^{n}$$

$$+ \frac{\omega^{2} z_{1} z_{2}}{(z_{1} - z_{2})^{2}} ((\omega z_{1} + \omega^{2} z_{2}) \exp(z_{1})$$

$$+ (-(1 - \omega - \omega^{2}) z_{1} + z_{2}) \exp(z_{2})) c^{n}$$

$$+ \frac{\omega^{2} z_{1} z_{2}}{(z_{1} - z_{2})^{3}} ((-\omega z_{1} - \omega^{2} z_{2}) (\exp(z_{1}) - \exp(z_{2}))$$

$$+ ((1 - \omega - \omega^{2}) z_{1} - z_{2}) (\exp(z_{1}) - \exp(z_{2}))) c^{n} .$$

$$(41)$$

Let us consider the stability given by the following eigenvalues in a wedge $\mathcal{W} = \{\zeta \in \mathbb{C} : | \arg(\zeta) \le \alpha\}$

For the stability we have $|S_m(z_1, z_2)| \leq 1$ whenever $z_1, z_2 \in \mathcal{W}_{\pi/2}$. The stability of the two iterations is given in the following theorem with respect to the stability.

Theorem 4. We have the following stability :

For S_1 we have a strong stability with $\max_{z_1 \leq 0, z_2 \in W_\alpha} |S_1(z_1, z_2)| \leq 1$, $\forall \alpha \in [0, \pi/2]$ with $0 \leq \omega \leq 1$.

For S_2 we have a strong stability with

$$\begin{split} \max_{z_1 \leq 0, z_2 \in W_\alpha} |S_2(z_1, z_2)| \leq 1 \ , \ \forall \ \alpha \in [0, \pi/2] \ with \ 0 \leq \omega \leq \left(\frac{1}{8 \ \tan^2(\alpha) + 1}\right)^{1/8} \ . \\ Proof. \ \text{We consider a fixed} \ z_1 = z, \ Re(z) < 0 \ \text{and} \ z_2 \to -\infty \ . \ \text{Then we obtain} \end{split}$$

$$S_1(z,\infty) = \omega^2 (1-e^z) ,$$
 (42)

 and

$$S_2(z,\infty) = \omega^4 (1 - (1 - z)e^z) .$$
(43)

If z = x + iy, x < 0 then : 1.) For S_1

$$|S_1(z,\infty)|^2 = \omega^4 |(1-2\exp(x)\cos y + \exp(2x))|, \qquad (44)$$

and hence

$$|S_1(z,\infty)| \le 1 \Leftrightarrow \omega^4 \le \left|\frac{1}{1-2\exp(x)\cos(y) + \exp(2x)}\right|.$$
(45)

Because of x < 0 and $y \in \mathbb{R}$ we could estimate $-2 \leq 2 \exp(x) \cos(y)$ and $\exp(2x) \geq 0$. From (45) we obtain $\omega \leq \frac{1}{\sqrt[4]{3}}$.

2.) For S_2

$$|S_2(z,\infty)|^2 = \omega^8 \{1 - 2\exp(x)[(1-x)\cos y + y\sin y] + \exp(2x)[(1-x)^2 + y^2]\},$$
(46)

after some calculations we could obtain

$$|S_2(z,\infty)| \le 1 \Leftrightarrow \exp(x) \le \left(\frac{1}{\omega^8} - 1\right) \frac{\exp(-x)}{(1-x)^2 + y^2} + 2\frac{|1-x| + |y|}{(1-x)^2 + y^2}, \quad (47)$$

we could estimate for x < 0 and $y \in \operatorname{I\!R} \frac{|1-x|+|y|}{(1-x)^2+y^2} \le 3/2$ and $\frac{1}{2\tan^2(\alpha)} < \frac{\exp(-x)}{(1-x)^2+y^2}$ where $\tan(\alpha) = y/x$.

Finally, we get the bound $\omega \leq \left(\frac{1}{8\tan^2(\alpha)+1}\right)^{1/8}$.

Remark 4. The stability is derived for ordinary differential equations with linear operators. For applications in linear partial differential equations we assume a discretization of the spatial operators, so that we obtain a system of linear ordinary differential equations. These equations can be treated as described below.

The stability for the damped iterative operator splitting method is given in the following theorem

Theorem 5. We have the following stability :

For S_1 we have a strong stability with $\max_{z_1 \leq 0, z_2 \in W_\alpha} |S_1(z_1, z_2)| \leq 1$, $\forall \alpha \in [0, \pi/2]$ with $\omega \leq 1/2$

Proof. We consider a fixed $z_1 = z$, Re(z) < 0 and $z_2 \to -\infty$. Then we obtain

$$S_1(z,\infty) = \frac{1-\omega}{\omega} (1-e^z) .$$
(48)

If z = x + iy, x < 0 then : 1.) For S_1

$$|S_1(z,\infty)|^2 = \left(\frac{1-\omega}{\omega}\right)^2 (1-2\exp(x)\cos(y) + \exp(2x)) , \qquad (49)$$

hence

$$|S_1(z,\infty)| \le 1 \Leftrightarrow \left(\frac{1-\omega}{\omega}\right)^2 \le \left|\frac{1}{1-2\exp(x)}\cos y + \exp(2x)\right|.$$
(50)

From (50) we obtain $0 \le \omega \le \frac{1}{2}$.

In the next section we derive an a posteriori error estimates for the iterative splitting methods, starting with different initial-solutions.

5 A posteriori error-estimates

We consider the a posteriori error-estimates for the beginning time iterations. We can derive the following theorem for the a posteriori error-estimates :

Theorem 6. Let us consider the iterative method, that starts with the following initial condition

case $A : c_{i-1}(t) = 0$

$$c_2 - c_1 = ||B||\tau + O(\tau^2), \qquad (51)$$

case $B: c_{i-1}(t) = c_n$

$$c_2 - c_1 = ||BA + B||\tau^2/2 + O(\tau^3), \qquad (52)$$

case $C: c_{i-1}(t) = exp(B(t-t_n))exp(A(t-t_n))$ (pre-step with A-B splitting method)

$$c_2 - c_1 = ||[A, B]||\tau^2/2 + O(\tau^3) , \qquad (53)$$

Proof. We apply the equation (35) and (36) and deal with $c_{i-1}(s) = 0$. So the first iteration c_1 is given as :

$$c_1(t) = \exp(A(t - t_n)) c_n$$
, (54)

The second iteration is given as :

$$c_2(t) = \exp(B(t - t_n)) \left(\int_{t_n}^t \exp(-B(s - t_n))A \exp(A(s - t_n)) \, dx + c_n \right) ,$$
(55)

The Taylor-expansion for the 2 functions leads to

$$c_1(t) = (I + A\tau + \frac{\tau^2}{2!}A^2)c_n + O(\tau^3) , \qquad (56)$$

 and

$$c_2(t) = (I + B\tau + \frac{\tau^2}{2!}B^2 + A\tau + A^2\frac{\tau^2}{2!} + BA\frac{\tau^2}{2!})c_n + O(\tau^3) , \qquad (57)$$

Subtracting the approximations we obtain :

$$||c_2 - c_1|| \le ||B||\tau c_n + O(\tau^2) , \qquad (58)$$

6 Discretization methods

For the discretization methods we apply higher order methods in time and space. This is important to support the higher order splitting methods.

6.1 Time-discretization methods

We deal with higher order time-discretization methods. Therefore we propose the Runge-Kutta and BDF-methods as adapted time-discretization methods to reach higher order results.

For the time-discretization we use the following higher order discretization methods.

Runge-Kutta method

We use the implicit trapezoidal rule:

$$\begin{array}{c|c} 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline \frac{1}{2} & \frac{1}{2} \end{array}$$
(59)

Further more we use the following Gauß Runge-Kutta method :

$$\frac{\frac{1}{2} - \frac{\sqrt{3}}{6}}{\frac{1}{2} + \frac{\sqrt{3}}{6}} \frac{\frac{1}{4}}{\frac{1}{4} - \frac{\sqrt{3}}{6}}{\frac{1}{2} + \frac{\sqrt{3}}{6}} \frac{\frac{1}{4}}{\frac{1}{2}} \frac{\frac{1}{2}}{\frac{1}{2}}$$
(60)

To use this Runge-Kutta methods with our operator-splitting method we have to take into account that we solve in each iteration step equations of the form $\partial_t u_i = Au_i + b$. Where $b = Bu_{i-1}$ is a discrete function as we only have a discrete solution for u_{i-1} .

For the implicit trapezoidal rule this is no problem, because we do not need the values at any sub-points. Where on the other hand for the Gauß method we need to now the values of b at the sub-points $t_0 + c_1 h$ and $t_0 + c_2 h$ with $c = (\frac{1}{2} - \frac{\sqrt{3}}{6}, \frac{1}{2} + \frac{\sqrt{3}}{6})^T$. Therefor we must interpolate b. To do so we choose the cubic spline functions.

Numerical experiments show that this works properly with non-stiff problems, but worth with stiff-problems.

BDF method

Because the higher order Gauß Runge-Kutta method combined with cubic spline interpolation does not work properly with stiff problems we use the following BDF method of order 3 which does not need any sub-points and therefor no interpolation is needed.

BDF3

$$1/k(11/6u^{n+2} - 3u^{n+1} + 3/2u^n - 1/3u^{n-1} = A(u^{n+3})$$
(61)

For the pre-stepping, i.e. to obtain u_1, u_2 , we use the above implicit trapezoidal rule.

6.2 Space-discretization methods

For the spatial discretization methods we apply finite difference methods for Cartesian grids and finite element methods for tridiagonal grids.

The higher order method in space are also important for preserving the convergence order in time.

So for the computations we can fulfill the same convergence order for time and space, see $O(\tau^m) \approx O(h^n)$, with τ is the time-step and h is the spatial-step, m is the discretization-order in time and n is the discretization order in space, see [19], [13], [14].

7 Numerical Results

We start with the nonlinear ordinary differential equations and compare the different splitting methods.

7.1 First test-example of a nonlinear ODE (Bernoulli-Equation)

We deal with a nonlinear ODE (Bernoulli-equation) and split into the linear and nonlinear operator.

We deal with the non linear Bernoulli-Equation:

$$\frac{\partial u(t)}{\partial t} = \lambda_1 u(t) + \lambda_2 u^n(t)$$
$$u(0) = 1$$

with the analytical solution

$$u(t) = \left[(1 + \frac{\lambda_2}{\lambda_1}) \exp(\lambda_1 t(1-n)) - \frac{\lambda_2}{\lambda_1}) \right]^{-\frac{1}{1-n}}$$
(62)
$$u(0) = u_1 \quad \text{(initial conditions)} (63)$$

 $u(0) = u_0$, (initial conditions) (.63)

We choose n=2 , $\lambda_1=-1,\,\lambda_2=-100$ and $h=10^{-2}$

We rewrite the equation-system (62)-(63) in operator notation, and end up with the following equations :

$$\partial_t u = A(u) + B(u) , \qquad (64)$$

$$u(0) = u_0,$$
 (65)

where $u(t) = (u_1(t), u_2(t))^T$ for $t \in [0, T]$. Our spitted operators are

$$A(u) = \lambda_1 u , B(u) = \lambda_2 u^m , \qquad (66)$$

with m = 2. The nonlinear example fulfills the non-commutative behavior $A'B - B'A \neq 0$.

Iterative	Number of	error
Steps	splitting-partitions	
2	1	7.3724e-001
2	2	2.7910e-002
5	1	4.1328e + 001
5	2	9.6601e-004
10	1	1.0578e-001
10	2	3.9777e-004
15	1	1.1933e-004
15	2	3.9782e-004
20	1	1.2081e-004
20	2	3.9782e-004

Table 1. Numerical results for the Bernoulli-Equation with the Iterative Operator Splitting method and BDF3.

7.2 Second Example (time-dependent equation)

In the second example we deal with a partial differential equation that is timedependent, see [1].

We deal with the time dependent 2-D equation:

$$\partial_t u(x, y, t) = u_{xx} + u_{yy} - 4(1 + y^2)e^{-t}e^{x + y^2}$$
(67)

$$u(x, y, 0) = e^{x+y^2}$$
 in $\Omega = [-1, 1] \times [-1, 1]$ (68)

$$u(x, y, t) = e^{-t} e^{x+y^2} \text{ on } \partial \Omega$$
(69)

(70)

with exact solution

$$u(x, y, t) = e^{-t}e^{x+y^2}$$
(71)

(72)

We choose the time interval [0,1] and again use Finite Differences for the space with $\Delta x = 2/19$.

We define our operators by splitting the plane into two parts.

We choose one splitting interval.

The maximum errors are given as Max-error = $\max_{i,j} u_{exact}(x_i, y_j, T) - u_{approx}(i\Delta x, j\Delta x, T)$

Iterative	Number of	Max-error
Steps	splitting-partitions	
1	1	2.7183e+000
2	1	8.2836e + 000
3	1	3.8714e + 000
4	1	2.5147e + 000
5	1	1.8295e + 000
10	1	6.8750e-001
15	1	2.5764 e - 001
20	1	8.7259e-002
25	1	2.5816e-002
30	1	5.3147 e-003
35	1	2.8774e-003

Table 2. Numerical results for the third example with the Iterative Operator Splitting method and BDF3 with $h = 10^{-1}$.

The relaxation error smooths as given in the following figures:



Fig. 1. The numerical results of the second example after 10 iterations (left) and 20 iterations (right).

7.3 Third example : Convection-reaction equation with sparsity pattern

We consider the one-dimensional convection-diffusion-reaction equation, where the reaction terms strong couple the equations.

It is given by

$$\begin{split} R\partial_t u + v\partial_x u - D\partial_{xx} u &= -\lambda u \text{, on } \Omega \times [t_0, t_{\text{end}}) \\ u(x, t_0) &= u_{\text{exact}}(x, t_0) \text{,} \\ u(0, t) &= u_{\text{exact}}(0, t) \text{, } u(L, t) = u_{\text{exact}}(L, t), \end{split}$$

We choose $x \in [0, 30]$, and $t \in [10^4, 2 \cdot 10^4]$. Furthermore we have $\lambda = 10^{-5}$, v = 0.001, D = 0.0001 and R = 1.0. The analytical solution is given by

$$u_{\text{exact}}(x,t) = \frac{1}{2\sqrt{D\pi t}} \exp(-\frac{(x-vt)^2}{4Dt}) \exp(-\lambda t) ,$$

To be out of the singular point of the exact solution, we start from the time-point $t_0 = 10^4$.

Our spitted operators are

$$A = \frac{D}{R}\partial_{xx}u , \ B = -\frac{1}{R}(\lambda u + v\partial_x u) .$$
(73)

For the spatial discretization we use the finite differences with $\Delta x = \frac{1}{10}$.

Iterative	Number of	error	error	error
Steps	splitting-partitions	x = 18	x = 20	x = 22
1	10	9.8993e-002	1.6331e-001	9.9054 e-002
2	10	9.5011e-003	1.6800e-002	8.0857 e-003
3	10	9.6209e-004	1.9782e-002	2.2922e-004
4	10	8.7208e-004	1.7100e-002	$1.5168\mathrm{e}{\text{-}003}$

Table 3. Numerical results for the second example with the Iterative Operator Splitting method and BDF3 with $h = 10^{-2}$.

8 Conclusions and Discussions

We present the convergence theory of the linear and nonlinear operator splitting method. The nonlinear theory deal with linearized operators and embedded into the linear theory. The stabilization is discussed by balancing the initial values of the iterative method by previous results or lower order operator-splitting methods. The benefit of such damped iterative methods are more stable methods without an influence coming from the initial values of the iteration. In experiments we verify our new methods in linear and nonlinear examples. The application to multi-physics problems show the benefit of the iterative operator splitting method as an efficient and accurate method for strong coupled equations. In the future we focus on the development of multi-level operator-splitting methods which is taken into account coarse and finer time-scales and apply the algorithms for nonlinear parabolic equations.



Fig. 2. Iterations 1 to 4 of the second example with the iterative splitting method and BDF3 $\,$



Fig. 3. Numerical result for the second example with the iterative splitting method and BDF3, left figure t = 0, right figure t = T.

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