

Iterative operator-splitting methods for Time-irreversible Systems: Theory and Application to Advection-Diffusion Equations

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Abstract. In this paper, we deduce higher order error bounds for iterative operator splitting methods for time-irreversible systems of linear advection-diffusion equations

$$\partial_t u = D\Delta u - \mathbf{v}\nabla u, \quad x \in \mathbb{R}^d, t \geq 0. \quad (1)$$

involving time-irreversible diffusion and a reversible advection part. We apply our analysis to bounded our advection operator with the diffusion operator (A -boundedness). We deduce a global error estimates which implies that any time-irreversible time-splitting methods retains its classical convergence of linear advection-diffusion equations, under some assumptions to the exact solution. Numerical results illustrate our theoretical results.

Keyword Iterative operator-splitting method, exponential splitting methods, advection-diffusion equations.

AMS subject classifications. 65L05, 65M125, 65J10.

1 Introduction

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

$$\partial_t u = D\Delta u - \mathbf{v}\nabla u = (A + B)u, \quad u(0) = u_0, \quad (2)$$

where involving that the advection operator can be bounded with the diffusion operator. For the analysis it is enough to have additional sufficiently often differentiable functions with bounded derivatives.

For the theoretical study we discuss the linear evolution equation as:

$$\partial_t c = (A + B)c, \quad c(0) = c_0, \quad (3)$$

where L, A and B are unbounded operators and B is an A -bounded operator.

The outline of the paper is as follows. The operator-splitting-methods are introduced in the Section 2. In Section 3, we discuss the error analysis of the different iterative methods and each benefit. In Section 4 we introduce the application of our methods for existing software tools. Finally we discuss future works in the area of iterative methods.

2 Iterative splitting method as a multi-product expansion

As numerical method we will imply a 1-stage iterative splitting scheme, also called Waveform-Relaxation method:

$$u_i(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i-1} ds, \quad (4)$$

where $i = 1, 2, 3, \dots$ and $u_0(t) = 0$.

As a second numerical method we will imply a 2-stage iterative splitting scheme :

$$u_i(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i-1} ds, \quad (5)$$

$$u_{i+1}(t) = \exp(Bt)u_0 + \int_0^t \exp(Bs)Au_i ds, \quad (6)$$

where $i = 1, 3, 5, \dots$ and $u_0(t) = 0$.

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

$$u_{i_k}(t) = \exp(At)u_0 + \int_0^t \exp(As)Bu_{i_k+J_{k-1}-1} ds, \quad (7)$$

$$u_{j_k+I_k}(t) = \exp(Bt)u_0 + \int_0^t \exp(Bs)Au_{j_k+I_k-1} ds, \quad (8)$$

where $i_k = 1, 2, 3, \dots, I_k$, $j_k = 1, 2, 3, \dots, J_k$, $k = 1, \dots, K$, I_1, \dots, I_K are the number of the iterations done with the A -operator, where J_1, \dots, J_K are the number of iterations done with the B -operator. The initialization is given as $u_0(t) = 0$ and $J_0 = 0$.

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

These iterative splitting methods can be written as a multi-product expansion, see section 3:

$$e^{\exp(A+B)} = \sum_{i=1}^n c_i \prod_{j=1}^{S_i} \exp hb_j B \exp ha_j B. \quad (9)$$

n is the number of multi iterations and S_i is the stage of each single product of the single iterative scheme.

The important time-irreversible splitting schemes are given in Table 2

2.1 Symplecticity of the iterative splitting scheme

We assume to have symplectic operators A , B for the iterative scheme.

By a transformation, one could rewrite an iterative scheme as an exponential splitting scheme, which is know to be symplectic, see [8].

Therefore we obtain also a symplectic splitting scheme.

method	order	single stages	multistage
Strang [17]	$p = 2$	$s = 2$	$n = 1$
Chin [1]	$p = 2$	$s = 2$	$n = 1$
Chin-Geiser [8]	$p = 4$	$s = 2$	$n = 2$
Suzuki [18]	$p = 6$	$s = 26$	$n = 1$

Table 1. Operator Splitting methods of order p , s compositions and n multilevel.

3 Error analysis for the general scheme

In the following, we derive our global error estimate for iterative operator splitting methods of the form (9) when applied to linear evolution equations (5).

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

$$\begin{aligned} \partial_t c(x, t) &= Ac(x, t) + Bc(x, t), \quad 0 < t \leq T \text{ and } x \in \Omega \\ c(x, 0) &= c_0(x) \quad x \in \Omega \\ c(x, t) &= c_1(x, t) \quad x \in \partial\Omega \times [0, T], \end{aligned} \quad (10)$$

where $A, B : D(\mathbf{X}) \rightarrow \mathbf{X}$ 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, see [11]:

$$\|B \exp((A + B)\tau)u_0\| \leq \kappa_1, \quad (11)$$

$$\|A \exp((A + B)\tau)u_0\| \leq \kappa_2, \quad (12)$$

Further we assume the estimation with ϕ -functions:

$$\|A \int_0^\tau \exp(As)ds\| \leq \tau C_1, \quad (13)$$

$$\|B \int_0^\tau \exp(Bs)ds\| \leq \tau C_2, \quad (14)$$

The we can bound our iterative operator splitting method as :

$$\|(S_i - \exp((A + B)\tau))\| \leq C\tau^i, \quad (15)$$

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. 1.) Exact solution:

The exact solutions can be derived with respect to variation of constants, see [19]:

$$\begin{aligned} c(t_n) &= \sum_{i=1}^n c_i \left(\exp hAc(t_{n-1}) + \sum_{k+1}^p I_k c(t_{n_1}) + R_{p+1}^{(1)} \right) \\ I_k &= \int_{\Delta_k} g_k(\tau) d\tau, R_{p+1}^{(1)} = \int_{\Delta_{p+1}} f_{p+1}(\tau) u(t_{n-1}) = \tau_{p+1} d\tau \end{aligned} \quad (16)$$

2.) Splitting operator (iterative splitting):

$$c(t_n) = \sum_{i=1}^n c_i \left(\exp hAc(t_{n-1}) + \sum_{k+1}^p I_k c(t_{n_1}) \right) \quad (17)$$

$$I_k = \int_{\Delta k} g_k(\tau) d\tau,$$

3.) Splitting operator (exponential splitting) , see [19].

4.) Local splitting error:

For e_i we have:

$$\|e_i\| \leq \|R_{p+1}^{(1)}\| = \left\| \int_{\Delta p+1} f_{p+1}(\tau) u(t_{n-1} = \tau_{p+1}) d\tau \right\| \quad (18)$$

$$\leq C\tau^i c(t^n),$$

where $\alpha = \min_{j=1}^i \{\alpha_j\}$ and $0 \leq \alpha_i < 1$.

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

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

but we reduce the convergence order

$$\|e_1\| = K \|B\| \tau^{\alpha_1} \|e_0\| + \mathcal{O}(\tau^{1+\alpha_1}) \quad (19)$$

and hence

$$\|e_2\| = K \|B\| \|e_0\| \tau^{1+\alpha_1+\alpha_2} + \mathcal{O}(\tau^{1+\alpha_1+\alpha_2}), \quad (20)$$

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

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.

3.1 Splitting of the Parabolic equations in a Hamiltonian setting

In the last years, the splitting to advection-diffusion equations gets important because of the more efficiency in computation.

Hamiltonian splitting

The advection-diffusion equation can be written as:

$$\partial_t c = -v \partial_x c + D \partial_{xx} c \quad (21)$$

$$(22)$$

we have $c = q_x$.

$$c_t = \frac{\delta H}{\delta p} = p \quad (23)$$

$$p_t = -\frac{\delta H}{\delta q} = -q_{xx} + \lambda q_x \quad (24)$$

with

$$H = \frac{1}{2} \int (p^2 + q_x^2 + 2\lambda q) dx. \quad (25)$$

Remark 3. The benefit of the Hamiltonian scheme is to obtain a kinetic and a potential part of the equation. Here the potential part can be solved as a linear elliptic equation, where the kinetic part is solved with ODE solvers, see also [1].

4 Numerical experiments

In this section we discuss the numerical experiments based on benchmark problems. We compare the standard splitting schemes, e.g. A-B splitting and the iterative schemes.

4.1 First Experiment

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

We deal with the following equation :

$$\partial_t u_1 = -\lambda_1 u_1 + \lambda_2 u_2, \quad (26)$$

$$\partial_t u_2 = \lambda_1 u_1 - \lambda_2 u_2, \quad (27)$$

$$u_1(0) = u_{10}, u_2(0) = u_{20} \text{ (initial conditions)}, \quad (28)$$

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 (26) in operator notation, we concentrate us to the following equations :

$$\partial_t u = A(t)u + B(t)u, \quad (29)$$

$$(30)$$

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 $\lambda_2(t) = t^2$.

and our splitted operators are

$$A = \begin{pmatrix} -\lambda_1 & \lambda_2 \\ 0 & 0 \end{pmatrix}, B = \begin{pmatrix} 0 & 0 \\ \lambda_1 & -\lambda_2 \end{pmatrix}. \quad (31)$$

The concrete parameters for the experiments are given as:

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

We apply the AB, Stang and 3rd order splitting and compared with the unsplit solutions:

1.) Unsplit :

$$c_{exact}(\tau) = \exp((A + B)\tau)c(t^n). \quad (32)$$

2.) A-B splitting

$$c_1(\tau) = \exp(A\tau) \exp(B\tau) c(t^n). \quad (33)$$

where we have a first order method, also known as AB splitting methods, see [3].

3.) Strang splitting

$$c_2(\tau) = \frac{1}{2}(\exp(At) \exp(Bt) + \exp(Bt) \exp(At)) \quad (34)$$

where we have a second order method, also known as parallel AB splitting method, see [3].

4.) 3rd order splitting

$$\begin{aligned} c_3(\tau) = & \frac{1}{6}(\exp(At) \exp(Bt) \exp(At) + \exp(Bt) \exp(At) \exp(At)) \quad (35) \\ & + \exp(Bt) \exp(Bt) \exp(At) + \exp(At) \exp(At) \exp(Bt) \\ & + \exp(At) \exp(Bt) \exp(Bt) + \exp(Bt) \exp(At) \exp(Bt) \end{aligned}$$

where the solution is derived of the iterative splitting methods.

The L_1 -error is computed as:

$$err_{num} = \sum_{k=1}^N |u_{exact}(t_k) - u_{num}(t_k)| \quad (36)$$

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

number of time partitions	err_1 (2nd order)	err_2 (2nd order)	err_1 (3rd order)	err_2 (3rd order)
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	6.6759e-008

Table 2. Numerical results for the first example with the iterative splitting method and 2nd- and 3rd-order method.

Remark 4. Our numerical results based on higher order iterative schemes in closed formulations. Table 2 presents the results in which the 3rd order methods can achieve more accurate results. The numerical results show that the splitting error decreases as long as the used Pade approximations 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 .

4.2 Second Experiment

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

We deal with the following equation :

$$\partial_t u_1 = -\lambda_1(t)u_1 + \lambda_2(t)u_2 , \quad (37)$$

$$\partial_t u_2 = \lambda_1(t)u_1 - \lambda_2(t)u_2 , \quad (38)$$

$$u_1(0) = u_{10} , u_2(0) = u_{20} \text{ (initial conditions) } , \quad (39)$$

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 (37) in operator notation, we concentrate us to the following equations :

$$\partial_t u = A(t)u + B(t)u , \quad (40)$$

$$(41)$$

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 $\lambda_2(t) = t^2$.

and our splitted operators are

$$At = \begin{pmatrix} -\lambda_1(t) & \lambda_2(t) \\ 0 & 0 \end{pmatrix} , Bt = \begin{pmatrix} 0 & 0 \\ \lambda_1(t) & -\lambda_2(t) \end{pmatrix} . \quad (42)$$

For the equation (37), we could apply a higher order Pade approximation, e.g. 3rd order.

We apply first the sequential splitting and the iterative operator-splitting, further we combine them be 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.

number of time partitions	err_1 (2nd order)	err_2 (2nd order)	err_1 (3rd order)	err_2 (3rd order)
1	4.5321e-002	3.6077e-003	4.5321e-002	3.6077e-003
10	4.6126e-004	3.6077e-003	4.6126e-004	3.6077e-003

Table 3. Numerical results for the second example with the iterative splitting method and 2nd- and 3rd-order method.

4.3 Third experiment

We deal with the 2-dimensional advection-diffusion equation and periodic boundary conditions

$$\begin{aligned}\partial_t u &= -\mathbf{v}\nabla u + D\Delta u, \\ &= -v_x \frac{\partial u}{\partial x} - v_y \frac{\partial u}{\partial y} + D \frac{\partial^2 u}{\partial x^2} + D \frac{\partial^2 u}{\partial y^2}, \\ u(\mathbf{x}, \mathbf{t}_0) &= u_0(\mathbf{x}),\end{aligned}$$

with the parameters

$$\begin{aligned}v_x &= v_y = 1 \\ D &= 0.01 \\ t_0 &= 0.25.\end{aligned}$$

The given advection-diffusion problem has an analytical solution

$$u_a(\mathbf{x}, t) = \frac{1}{t} \exp\left(\frac{-(\mathbf{x} - \mathbf{v}t)^2}{4Dt}\right)$$

which we will use as a convenient initial function:

$$u(\mathbf{x}, t_0) = u_a(\mathbf{x}, t_0)$$

We apply dimensional splitting to our problem

$$\frac{\partial u}{\partial t} = A_x u + A_y u$$

where

$$A_x = -v_x \frac{\partial u}{\partial x} + D \frac{\partial^2 u}{\partial x^2}.$$

We use a 1st order upwind scheme for $\frac{\partial}{\partial x}$ and a 2nd order central difference scheme for $\frac{\partial^2}{\partial x^2}$. By introducing the artificial diffusion constant $D_x = D - \frac{v_x \Delta x}{2}$ we achieve a 2nd order finite difference scheme

$$\begin{aligned}L_x u(x) &= -v_x \frac{u(x) - u(x - \Delta x)}{\Delta x} \\ &+ D_x \frac{u(x + \Delta x) + u(x) + u(x - \Delta x)}{\Delta x^2}.\end{aligned}$$

because the new diffusion constant eliminates the first order error (i.e. the numerical viscosity) of the Taylor expansion of the upwind scheme. $L_y u$ is derived in the same way.

We apply a BDF5 method to gain 5th order accuracy in time:¹

$$L_t u(t) = \frac{1}{\Delta t} \left(\frac{137}{60} u(t + \Delta t) - 5u(t) + 5u(t - \Delta t) - \frac{10}{3} u(t - 2\Delta t) + \frac{5}{4} u(t - 3\Delta t) - \frac{1}{5} u(t - 4\Delta t) \right). \quad (43)$$

Our aim is to compare the iterative splitting method with AB-splitting. Since $[A_x, A_y] = 0$ there is no splitting-error for the AB-splitting and therefore we cannot expect to achieve better results with the iterative splitting in terms of general numerical accuracy. Instead we will show that the iterative splitting out competes AB-splitting regarding the computational effort and round-off-errors. But first there are some remarks which have to be made concerning the special behavior of both methods when combined with high-order Runge-Kutta and BDF methods.

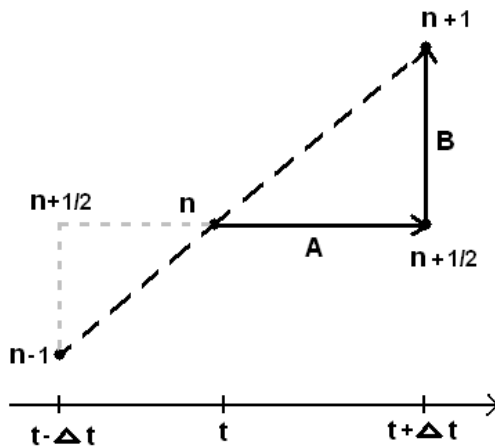


Fig. 1. Principle of the AB-Splitting.

Splitting and schemes of high order in time Concerning AB-Splitting:

The principle of AB-splitting is well known and simple. The equation $\frac{du}{dt} =$

¹ Please note that the dependencies of $u(\mathbf{x}, t)$ are suppressed for the sake of simplicity.

$Au + Bu$ is broken up into

$$\begin{aligned}\frac{du^{n+1/2}}{dt} &= Au^{n+1/2} \\ \frac{du^{n+1}}{dt} &= Bu^{n+1}\end{aligned}$$

which are connected via $u^{n+1}(t) = u^{n+1/2}(t + \Delta t)$. This is pointed out in figure (1). AB-splitting works very well for any given one-step method like the Crank-Nicholson-Scheme. Not taking into account the splitting-error (which is an error in time) it is also compatible with high order schemes such as explicit/implicit Runge-Kutta-schemes.

Things look different if one tries to use a multi-step method like the implicit BDF or the explicit Adams method with AB-splitting, these cannot be properly applied as is shown by the following example:

Choose for instance a BDF2 method which, in case of $du/dt = f(u)$, has the scheme

$$\frac{3}{2}u(t + \Delta t) - 2u(t) + \frac{1}{2}u(t - \Delta t) = \Delta t f(u(t + \Delta t)).$$

So the first step of the AB-splitting looks like:

$$\frac{3}{2}u^{n+1/2}(t + \Delta t) - 2u^{n+1/2}(t) + \frac{1}{2}u^{n+1/2}(t - \Delta t) = \Delta t Au(t + \Delta t)$$

Clearly $u^{n+1/2}(t) = u^n(t)$ but what is $u^{n+1/2}(t - \Delta t)$? This is also shown in figure (1) and it is obvious that we won't have knowledge about $u^{n+1/2}(t - \Delta t)$ unless we compute it separately which means additional computational effort. This overhead even increases dramatically when we move to a multi-step method of higher order.

The mentioned problems with the AB-splitting will not occur with a higher order Runge-Kutta method since only knowledge of $u^n(t)$ is needed.

Remarks about the iterative splitting: The BDF methods apply very well to the iterative splitting. Let us recall at this point that this method, although being a real splitting scheme, always remains a combination of the operators A and B so no steps have to be done into one direction only ².

In particular we do a subdivision of our given time-discretization $t_j = t_0 + j\Delta t$ into I parts. So we have subintervals $t_{j,i} = t_j + i\Delta t/I$, $0 \leq i \leq I$ on which we solve the following equations iteratively:

² As we will see there is an exception to this.

$$\frac{du^{i/I}}{dt} = Au^{i/I} + Bu^{(i-1)/I} \quad (44)$$

$$\frac{du^{(i+1)/I}}{dt} = Au^{i/I} + Bu^{(i+1)/I} \quad (45)$$

$$(46)$$

$u^{-1/I}$ is either 0 or a reasonable approximation³ while $u^0 = u(t_j)$ and $u^1 = u(t_j + \Delta t)$. The crucial point here is that we only know our approximations at given times which don't happen to be the times at which a Runge-Kutta method needs to know them. Therefore, in case of a RK method, the values of the approximations have to be interpolated with at least the accuracy one wishes to attain with the splitting and this means a lot of additional computational effort. We may summarize our results now in table 4.3 that shows which methods are practicable for each kind of splitting scheme.⁴

	low order s.s.m.	high order s.s.m.	m.s.m.
AB-splitting	X	X	-
Iterative splitting	X	-	X

Table 4. Practicability of single- and multi-step methods (s.s.m: single-step methods, m.s.m. multi-step methods).

Numerical results After resolving the technical aspects of this issue we can now proceed to the actual computations. The question which arises is which of the splitting methods has the least computational effort since we can expect them to solve the problem with more or less the same accuracy if we use practicable methods with equal order because $[A_x, B_x] = 0$. We tested the dimensional splitting of the 2d-advection-diffusion equation with the AB-splitting combined with a 5th order RK method after Dormand and Prince and with the iterative splitting in conjunction with a BDF5 scheme. We used 40×40 - and 80×80 -grids and completed n_t time-steps with each of which subdivided into 10 smaller steps

³ In fact the order of the approximation is not of much importance if we fulfill a sufficient number of iterations. In case of $u^{-1/I} = 0$ we have the exception that a step in A-direction is done while B is left out. The error of this step vanishes after a few but mostly only one iteration

⁴ In favor of the iterative splitting scheme take also into the account that AB-splitting may be used along with the mentioned high order methods but cannot maintain the order if $[A, B] \neq 0$ while the iterative splitting re-establishes the maximum order of the scheme when a sufficient number of iterations is done.

until we reached time $t_{end} = 0.6$ which is sufficient to see the main effects. The iterative splitting was done with 2 iterations which was already enough to attain the desired order. In tables 5 and 6 the errors at time t_{end} and the computation times are shown.

Number of steps	Error AB	Error It.spl.	AB computation time	It. spl. computation time
5	0.1133	0.1154	0.203 s	0.141 s
10	0.1114	0.1081	0.500 s	0.312 s
30	0.1074	0.1072	1.391 s	0.907 s
50	0.1075	0.1074	2.719 s	1.594 s

Table 5. Errors and computation times of AB-splitting and iterative splitting for a 40×40 -grid.

Number of steps	Error AB	Error It.spl.	AB computation time	It. spl. computation time
5	0.0288	0.0621	0.812 s	0.500 s
10	0.0276	0.0285	2.031 s	1.266 s
30	0.0268	0.0267	6.109 s	4.000 s
50	0.0265	0.0265	12.703 s	7.688 s

Table 6. Errors and computation times of AB-splitting and iterative splitting for a 80×80 -grid.

As we can see, the error of the iterative splitting reaches the AB-splitting error after a certain number of time-steps and stays below it for all additional steps we accomplish. Of course the error cannot sink under a certain amount which is governed by the spatial discretization. It is to be noticed that while the computation time used for the iterative splitting is always about 20%-40% less than that of the AB-splitting⁵ the accuracy is, with a sufficient number of time-steps, slightly better than that of the AB-splitting. This is due to the roundoff error which is higher for the Runge-Kutta method because of the greater amount of basic operations needed to compute the RK steps.

A future task will be to introduce non-commuting operators in order to show the superiority of the iterative splitting over the AB-splitting when the order in time is reduced due to the splitting error.

⁵ The code for both methods is kept in the simplest possible form.

5 Conclusions and Discussions

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

References

1. S.A. Chin and C.R. Chen. *Gradient symplectic algorithms for solving the Schrödinger equation with time-dependent potentials*. Journal of Chemical Physics, 117(4), 1409-1415 (2002).
2. S.A. Chin. *Multi-product splitting and Runge-Kutta-Nyström integrators*. ArXiv:0809.0914; Applied Numerical Mathematics, under review (2008).
3. I. Farago, J. Geiser. *Iterative Operator-Splitting Methods for Linear Problems*. Preprint No. 1043 of the Weierstass Institute for Applied Analysis and Stochastics, (2005) 1-18. International Journal of Computational Science and Engineering, accepted September 2007.
4. J. Geiser. *Higher order splitting methods for differential equations: Theory and applications of a fourth order method*. Numerical Mathematics: Theory, Methods and Applications. Global Science Press, Hong Kong, China, accepted, April 2008.
5. J. Geiser and L. Noack. *Iterative operator-splitting methods for nonlinear differential equations and applications of deposition processes*. Preprint 2008-4, Humboldt University of Berlin, Department of Mathematics, Germany, 2008.
6. J. Geiser and Chr. Kravvaritis. *A Domain Decomposition method based on iterative Operator Splitting method*. Applied Numerical Mathematics, 59, 608-623, 2009.
7. J. Geiser and Chr. Kravvaritis. *Overlapping operator splitting methods and applications in stiff differential equations*. Special issue: Novel Difference and Hyprod Methods for Differential and Integro-Differential Equations and Applications, Guest editors: Qin Sheng and Johnny Henderson, Neural, Parallel, and Scientific Computations (NPSC), 16, 189-200, 2008.
8. J. Geiser and S. Chin. *Multi-product expansion, Suzuki's method and the Magnus integrator for solving time-dependent problems*. Preprint 2009-4, Humboldt University of Berlin, Department of Mathematics, Germany, 2009.
9. R. Glowinski. *Numerical methods for fluids*. Handbook of Numerical Analysis, Gen. eds. P.G. Ciarlet, J. Lions, Vol. IX, North-Holland Elsevier, Amsterdam, The Netherlands, 2003.
10. M. Hochbruck and A. Ostermann. *Explicit Exponential Runge-Kutta Methods for Semilinear Parabolic Problems*. SIAM Journal on Numerical Analysis, Vol. 43, Iss. 3, 1069-1090, 2005.
11. E. Hansen and A. Ostermann. *Exponential splitting for unbounded operators*. Mathematics of Computation, accepted, 2008.
12. T. Jahnke and C. Lubich. *Error bounds for exponential operator splittings*. BIT Numerical Mathematics, 40:4, 735-745, 2000.

13. J. Kanney, C. Miller and C. Kelley. *Convergence of iterative split-operator approaches for approximating nonlinear reactive transport problems*. Advances in Water Resources, 26:247–261, 2003.
14. C.T. Kelly. *Iterative Methods for Linear and Nonlinear Equations*. Frontiers in Applied Mathematics, SIAM, Philadelphia, USA, 1995.
15. G.I. Marchuk. *Some applications of splitting-up methods to the solution of problems in mathematical physics*. Aplikace Matematiky, 1, 103-132, 1968.
16. A. Rouhi and J. Wright. *A new operator splitting method for the numerical solution of partial differential equations*. Computer Physics Communication, 85, 18–28, 1995.
17. G. Strang. *On the construction and comparison of difference schemes*. SIAM J. Numer. Anal., 5, 506-517, 1968.
18. M. Suzuki. *General Decomposition Theory of Ordered Exponentials*. Proc. Japan Acad., vol. 69, Ser. B, 161 (1993).
19. M. Thalhammer. *High-order exponential operator splitting methods for time-dependent Schrödinger equations*. Siam J. Num. Anal., vol. 46, No.4, 2022-2038, 2008.
20. S. Vandewalle. *Parallel Multigrid Waveform Relaxation for Parabolic Problems*. Teubner Skripten zur Numerik, B.G. Teubner Stuttgart, 1993.