Application of Operator Splitting to Solve Reaction-Diffusion Equations*

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Abstract

Approximate solutions of systems of semilinear ordinary differential equations obtained by different splitting methods are investigated. The local error in the numerical solution of such semilinear problems is evaluated. The order of different splitting methods coupled with numerical methods of different order is calculated symbolically and on a test problem –the spatially discretized Fisher equation– numerically.

1 Introduction

Splitting methods have been fruitfully used to solve large systems of partial differential equations. To find the exact solution of a given problem in practice is usually impossible. We can use numerical methods to obtain an approximate solution of the equations, although to solve the discretized model can still be very difficult. Reaction-diffusion models or models of transport processes have a structure that allows a natural decomposition of the equations, thus provide the opportunity to apply operator splitting schemes. Splitting methods help us reduce the complexity of the system and reduce computational time. With splitting it is possible to handle stiff terms separately and to solve each subproblem with a suitable numerical method chosen to the corresponding operator. Although our motivations come from the investigation of reaction-diffusion equations, this paper considers the case of finite dimensional problems, we study systems of ordinary differential

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*This paper is in final form and no version of it will be submitted for publication elsewhere.

equations which can be split into a couple of a linear and a nonlinear subproblem. Such a system of ODEs may come from spatial discretization of a system of partial differential equations describing reaction-diffusion processes. To solve a problem in practice we use operator splitting and numerical schemes which we will call the *combined method*. The use of operator splitting as well as the numerical methods result in some error in the solution. The error generated purely by splitting is called *splitting error*. This is the difference of the exact solution and the approximate solution obtained by splitting (assumed that we know the exact solutions of the subproblems). Combined methods can generate both splitting error and *numerical error*. The study of this common effect on the solution is our main concern in this paper. Detailed study on the interaction of operator splitting and numerical schemes for *linear* problems can be found in [Csomós and Faragó]. They classify the errors that can occur using splitting methods and numerical schemes, give theoretical and numerical results on the order of the combined method for linear problems. Our aim is to characterize the error of this combined method therefore we calculate the order of the combined method for a *nonlinear* problem. We analyze the order of the error in the light of the characteristics of the splitting error and the numerical error. [Sanz-Serna] and [Hundsdorfer and Verwer] discuss the splitting error in a general framework. Here we intend to rigorously analyze the interaction of splitting error and numerical error in the case of a system of nonlinear ODE that can be split into a linear and a nonlinear subproblem.The structure of our paper is as follows. In section 2 we introduce the basic idea and notions of operator splitting. In Section 3 we calculate the order of the combined method for the type of problems mentioned above: split into linear and nonlinear subproblems. In Section 4 we introduce the Fisher equation and recall some known results on it. We show how we apply splitting to solve the Fisher equation. Section 5 contains the numerical results on the Fisher equation.

2 Operator splitting

2.1 The basic idea

Let us consider the following finite dimensional problem:

$$u'(t) = F(u(t)), \quad u(0) = u_0. \tag{1}$$

Let X be a finite dimensional normed vector space and $F : X \to X$ be an operator with domain of definition $D(F)$ and $u_0 \in D(F)$. Suppose that F can be written as

the sum of a linear and a nonlinear operator, successively: $F = A + R$.

The most simple type of operator splitting is the sequential splitting. In this case the split problem is:

$$u_1'(t) = Au_1(t), \quad u_1(0) = u_0, \tag{2}$$

$$u_2'(t) = R(u_2(t)), \quad u_2(0) = u_1(\tau). \tag{3}$$

The basic idea of splitting is to decompose the operator on the right hand side into the sum of simpler operators, and to solve the subproblems corresponding to the operators successively in each time step. More precisely, we solve the equation only with operator A until time τ (as if only the subprocess represented by A were present) and the solution in time τ will be the initial condition of the equation with R. It means that we return to the initial time and solve the equation with R as well. The solution of the second equation in time τ is called the approximate solution of the original problem in time τ. This procedure is then repeated on the interval $[\tau, 2\tau]$ etc. Thus, the simpler subproblems are connected to each other through the initial conditions. It is clear, that the numerical treatment of the separate subproblems is simpler. The most significant advantage of splitting is that we can exploit the special properties of the operators of the different subproblems and apply the most suitable numerical method for each of them. Thus we can obtain a more accurate solution in a shorter time.

We remark that the method can be used fruitfully in large models, for example global models of air pollution transport, or combustion or metabolic models, where the number of predicted variables is large and the number of the processes represented in the models is large. We refer to the work [Lagzi et al.] on air pollution models with application of operator splitting. Certain type of operator splittings allows the parallelization of the problem which is also advantageous in reducing the computational time of large system.

2.2 Splitting schemes

We can define the different splitting methods by solving the subproblems successively in different orders and for different time lengths. The above described simplest scheme is called *sequential* splitting (SEQ). We solve the subproblems one after another using the same time length τ, schematically $S_2(\tau)S_1(\tau)$, where S_1 and S_2 denote the solution operator corresponding to (2) and (3) respectively. In *Marchuk–Strang* splitting (MS) we usually solve the subproblem with A for

time length $\tau/2$ then solve the other one with R for time length τ and solve with A again for time length $\tau/2$. Schematically $S_1(\tau/2)S_2(\tau)S_1(\tau/2)$. In the case of reaction-diffusion problems R is chosen to be the operator representing chemical reactions, in general the operator that is stiff or nonlinear. In this given order we need to solve the second subproblem only one time which can be of importance given the operator's properties. See more in [Marchuk] and [Strang]. In *weighted sequential* splitting the solution in the next time step is a weighted average of the results of the two possible sequential splittings $S_1(\tau)S_2(\tau)$ and $S_2(\tau)S_1(\tau)$. In the special case of *symmetrically weighted* splitting (SW) we take the arithmetic mean of the results: $(S_1(\tau)S_2(\tau) + S_2(\tau)S_1(\tau))/2$. The extra work with MS and SW splittings benefits in second order accuracy compared to the first order of SEQ splitting. The nonsymmetric weighted splitting is of order one. In later sections we investigate the SEQ, the MS and the SW splittings coupled with four different numerical methods, all of different orders.

2.3 Splitting error, order of splitting

We discretize (1) in time in an equidistant manner with time step τ. If we know the exact solutions of (2) and (3) we can generate an approximate solution to the original full problem (1). In this case error originated only from operator splitting can arise. Let us denote the exact solution by u and the approximate solution by $\tilde{u}_{spl}$.

Definition 1 *The local splitting error at the end of the first time step is*

$$e_{spl}(\tau) := u(\tau) - \tilde{u}_{spl}(\tau).$$

Here both solutions start from the common initial value u_0. Naturally the local splitting error can be defined at any point of time, if $u(t) = \tilde{u}_{spl}(t)$ then $u(t+\tau) - \tilde{u}_{spl}(t+\tau)$ is the local splitting error at $t+\tau$.

Definition 2 *We say that a given operator splitting is of order p if*

$$e_{spl}(\tau) = O(\tau^{p+1})$$

In general – infinite dimensional case included – for linear bounded operators it can be shown by Taylor expansion that the local order of SEQ equals 1 since the error becomes $e_{spl}(\tau) = K\tau^2 + O(\tau^3)$. For nonlinear operators we need the definition of the *Lie-operator* and we can perform the analysis with Taylor expansion using the Lie-operators. We refer to [Hundsdorfer and Verwer] for detailed

derivation of the nonlinear case. From the literature on operator splitting it is well known that the MS provides second order accuracy, so does the SW splitting, see [Faragó and Havasi, 1] and [Faragó and Havasi, 2].

3   Order of combined methods

When we solve problem (1) we can use some kind of splitting but we can not avoid applying some numerical method as well. So in practice we use a combined method, a mixture of operator splitting and a numerical scheme and generate an approximate solution. Our aim is to calculate the order of the local error of this combined method for different splittings coupled with different numerical methods. To do this we will use the Taylor-formula in arbitrary normed vector spaces. The Taylor-formula can be found in e. g. [Komornik]. Here we cite the theorem:

Theorem 1 *Let X_1 and X_2 be normed vector spaces. If $f : X_1 \to X_2$ is n times differentiable at $a \in X_1$ and $\delta \to 0$, then*

$$f(a+\delta) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!} \delta^k + \varepsilon(\delta)\|\delta\|^n$$

where $\delta^k := (\delta, ..., \delta) \in X^k$ and $\lim_{\delta \to 0} \varepsilon(\delta) = 0$.

Suppose that u is the solution of the equation:

$$u'(t) = Au(t) + R(u(t)), \quad u(t_0) = u_0. \tag{4}$$

Remark 1 *If we consider (4) to be originated from a PDE describing a reaction-diffusion process then the linear A is the spatially discretized analogue of the operator representing diffusion and R is the analogue for chemical reactions (in many practical cases a polynomial). The investigation of a continuous reaction-diffusion model is complicated due to the unboundedness of diffusion.*

Let $X = \mathbb{R}^d$ and $A \in \mathbb{R}^{d \times d}$ a matrix. Thus the mapping $x \mapsto A \cdot x$ is a bounded linear operator defined on the whole set $\mathbb{R}^d$, it is infinitely many times differentiable and $A'(x) = A$ for every $x \in \mathbb{R}^d$. We suppose that $R : \mathbb{R}^d \to \mathbb{R}^d$ is a differentiable non-linear mapping, for the following derivations we need R to be at least two times differentiable. Henceforth we also assume that (4) has a sufficiently smooth solution $u : \mathbb{R}^+ \to \mathbb{R}^d$. Based on (4) and the chain-rule u' is a differentiable function, thus $u''(t) \in \mathbb{R}^d$ exists for all $t > 0$.

Under these above conditions we can use the Taylor-formula with $X_1 = \mathbb{R}$ and $X_2 = \mathbb{R}^d$ for u in time t_0, it gives

$$u_\tau := u(t_0 + \tau) = u(t_0) + u'(t_0)\tau + \frac{1}{2}u''(t_0)\tau^2 + \varepsilon(\tau)\tau^2$$

with $\lim_{\tau \to 0} \varepsilon(\tau) = 0$. We will neglect the norm as we did here since u acts on $\mathbb{R}^+$ so τ denotes a positive real number. $u'(t_0)$ is given by (4), we get $u''(t_0)$ by differentiation of (4):

$$u''(t_0) = A'(u(t_0)) \circ u'(t_0) + R'(u(t_0))u'(t_0) = Au'(t_0) + R'(u(t_0))u'(t_0) =$$

$$= A^2 u(t_0) + R(u(t_0)) + R'(u(t_0))Au(t_0) + R'(u(t_0))R(u(t_0)).$$

We can express u_τ with the known value of $u_0 = u(t_0)$ as:

$$u_\tau = u_0 + \big(Au_0 + R(u_0)\big)\tau + \tag{5}$$

$$+ \frac{1}{2}\Big(A^2 u_0 + AR(u_0) + R'(u_0)Au_0 + R'(u_0)R(u_0)\Big)\tau^2 + \varepsilon(\tau)\tau^2$$

with $\lim_{\tau \to 0} \varepsilon(\tau) = 0$.

Definition 3 *The local error of a combined method at $t_0 + \tau$ is:*

$$e_{loc}(t_0 + \tau) := u(t_0 + \tau) - \tilde{u}(t_0 + \tau) = u_\tau - \tilde{u}_\tau,$$

assuming that $u(t_0) = \tilde{u}(t_0)$, where $\tilde{u}$ is the approximate solution generated by the combined method. We say that a given combined method is of order s if

$$e_{loc}(t_0 + \tau) = O(\tau^{s+1}).$$

In the following examinations we will take the time step of the numerical method equal to the splitting time step.

Theorem 2 *The sequential splitting combined with the first order Euler forward scheme provides a first order method.*

Proof. The proof will be given in two steps.

Step 1: linear-nonlinear case. If we use SEQ starting with the nonlinear problem corresponding to R combined with Euler forward method for both subproblems we get:

$$\begin{cases} u^* = u_0 + \tau R(u_0) \\ \tilde{u}_\tau = u^* + \tau Au^* \end{cases}$$

where u^* is the intermediate value of u. The approximation of the solution is:

$$\tilde{u}_\tau = u^* + \tau A u^* = u_0 + \tau R(u_0) + \tau A(u_0 + \tau R(u_0)).$$

Since A is linear we have:

$$\tilde{u}_\tau = u_0 + \tau R(u_0) + \tau A u_0 + \tau^2 A R(u_0). \tag{6}$$

The local error generated in this step of length τ is the difference of (5) and (6):

$$u_\tau - \tilde{u}_\tau = \left(A^2 u_0 - A R(u_0) + R'(u_0) A u_0 + R'(u_0) R(u_0) \right) \frac{\tau^2}{2} + \varepsilon(\tau) \tau^2.$$

Step 2: nonlinear-linear case. If we use SEQ starting with the linear problem corresponding to A combined with Euler forward method for both subproblems we get:

$$\begin{cases} u^* = u_0 + \tau A u_0 \\ \tilde{u}_\tau = u^* + \tau R(u^*). \end{cases}$$

The approximation of the solution is:

$$\tilde{u}_\tau = u^* + \tau R(u^*) = u_0 + \tau A u_0 + \tau R(u_0 + \tau A u_0).$$

Here we apply the Taylor-formula with $X_1 = X_2 = \mathbb{R}^d$ for the function R, the point "a" is u_0 and the *increment* δ equals to $\tau A u_0$ now. We get

$$R(u_0 + \tau A u_0) = R(u_0) + R'(u_0) \tau A u_0 + \varepsilon_1(\tau A u_0) \| \tau A u_0 \|.$$

With

$$\varepsilon(\tau) := \varepsilon_1(\tau A u_0) \| A u_0 \|$$

we obtain

$$R(u_0 + \tau A u_0) = R(u_0) + R'(u_0) \tau A u_0 + \varepsilon(\tau) \tau.$$

Then

$$\tilde{u}_\tau = u_0 + \tau A u_0 + \tau \left(R(u_0) + R'(u_0) \tau A u_0 + \varepsilon(\tau) \tau \right) =$$
$$= u_0 + \tau A u_0 + \tau R(u_0) + R'(u_0) \tau^2 A u_0 + \varepsilon(\tau) \tau^2.$$

Recall (5) here:

$$u_\tau = u_0 + \tau(A u_0 + R(u_0)) +$$
$$+ \left(A^2 u_0 + A R(u_0) + R'(u_0) A u_0 + R'(u_0) R(u_0) \right) \frac{\tau^2}{2} + \varepsilon(\tau) \tau^2.$$

Comparing this with the approximation we get:

$$u_\tau - \tilde{u}_\tau = \left(A^2 u_0 + AR(u_0) - R'(u_0)Au_0 + R'(u_0)R(u_0)\right)\frac{\tau^2}{2} + \varepsilon(\tau)\tau^2.$$

$\square$

Theorem 3 *SW combined with the first order Euler forward method provides a method of first order.*

Proof. Here we simply use the above results with some $\omega \in [0,1]$ parameter:

$$\tilde{u}_\tau = \omega\left(u_0 + \tau\left(R(u_0) + Au_0\right) + \tau^2 AR(u_0)\right) +$$

$$+(1-\omega)\left(u_0 + \tau\left(Au_0 + R(u_0)\right) + R'(u_0)\tau^2 Au_0\right) + \varepsilon(\tau)\tau^2 =$$

$$= u_0 + \tau\left(Au_0 + R(u_0)\right) + \left(\omega AR(u_0) + (1-\omega)(R'(u_0)Au_0)\right)\tau^2 + \varepsilon(\tau)\tau^2.$$

For the local error we have:

$$u_\tau - \tilde{u}_\tau =$$

$$= \left(A^2 u_0 + (1-2\omega)Au_0 R(u_0) + (2\omega-1)R'(u_0)Au_0 + R'(u_0)R(u_0)\right)\frac{\tau^2}{2} + \varepsilon(\tau)\tau^2.$$

It is clearly of first order. With $\omega = 1/2$ we have

$$u_\tau - \tilde{u}_\tau = \left(A^2 u_0 + R'(u_0)R(u_0)\right)\frac{\tau^2}{2} + \varepsilon(\tau)\tau^2.$$

$\square$

Remark 2 *Although the SW is of second order its combination with the first order Euler method provides only first order accuracy.*

The above derivation can be used to determine the order of combined methods with higher order numerical schemes. The method can be extended for schemes of arbitrary order although the calculations become very complicated as the order increases. As an example let us consider the improved Euler scheme which is of second order and combine it with SEQ:

Theorem 4 *The second order improved Euler scheme combined with SEQ provides a first order method.*

Proof. Again, the proof will be given in two steps.

Step 1: nonlinear-linear case.

$$\begin{cases} u^* = u_0 + \tau A(u_0 + \dfrac{\tau}{2}Au_0) \\ \tilde{u}_\tau = u^* + \tau R(u^* + \dfrac{\tau}{2}R(u^*)) \end{cases}$$

The approximation of the solution is:

$$\tilde{u}_\tau = u^* + \tau R\left(u^* + \frac{\tau}{2}R(u^*)\right) = u_0 + \tau A\left(u_0 + \frac{\tau}{2}Au_0\right) +$$

$$+\tau R\left(u_0 + \tau A\left(u_0 + \frac{\tau}{2}Au_0\right) + \frac{\tau}{2}R\left(u_0 + \tau A\left(u_0 + \frac{\tau}{2}Au_0\right)\right)\right) =$$

$$= u_0 + \tau Au_0 + \frac{\tau^2}{2}A^2u_0 + \tau R\left(u_0 + \underline{\tau\left(Au_0 + \frac{\tau}{2}A^2u_0 + \frac{1}{2}R\left(u_0 + \tau Au_0 + \frac{\tau^2}{2}A^2u_0\right)\right)}\right).$$

The underlined part is now the increment in the argument of R. The first order Taylor-expansion gives:

$$\tilde{u}_\tau = u_0 + \tau Au_0 + \frac{\tau^2}{2}A^2u_0 + \tau R(u_0) +$$

$$+\tau R'(u_0)\underline{\tau\left(Au_0 + \frac{\tau}{2}A^2u_0 + \frac{1}{2}R\left(u_0 + \tau Au_0 + \frac{\tau^2}{2}A^2u_0\right)\right)} + \varepsilon(\tau)\tau^2$$

expanding this we get

$$\tilde{u}_\tau = u_0 + \tau\left(Au_0 + R(u_0)\right) +$$

$$+\frac{\tau^2}{2}\left(A^2u_0 + 2R'(u_0)Au_0 + R'(u_0)R\left(u_0 + \underline{\tau Au_0 + \frac{\tau^2}{2}A^2u_0}\right)\right) +$$

$$+\frac{\tau^3}{2}R'(u_0)A^2u_0 + \varepsilon(\tau)\tau^2.$$

Taking the Taylor-expansion again, with the increment underlined:

$$\tilde{u}_\tau = u_0 + \tau\left(Au_0 + R(u_0)\right) +$$

$$+\frac{\tau^2}{2}\left(A^2u_0 + 2R'(u_0)Au_0 + R'(u_0)\left(R(u_0) + \tau R'(u_0)Au_0 + \frac{\tau^2}{2}R'(u_0)A^2u_0\right)\right) +$$

$$+\varepsilon(\tau)\tau^2 =$$

$$= u_0 + \tau\left(Au_0 + R(u_0)\right) + \frac{\tau^2}{2}\left(A^2 u_0 + 2R'(u_0)Au_0 + R'(u_0)R(u_0)\right) + \varepsilon(\tau)\tau^2.$$

The error becomes:

$$u_\tau - \tilde{u}_\tau = \left(AR(u_0) - R'(u_0)Au_0\right)\frac{\tau^2}{2} + \varepsilon(\tau)\tau^2.$$

Step 2: linear-nonlinear case.

$$\begin{cases} u^* = u_0 + \tau R(u_0 + \frac{\tau}{2}R(u_0)) \\ \tilde{u}_\tau = u^* + \tau A(u^* + \frac{\tau}{2}Au^*) \end{cases}$$

The approximation is:

$$\tilde{u}_\tau = u^* + \tau A\left(u^* + \frac{\tau}{2}Au^*\right).$$

Substituting the first equation:

$$\tilde{u}_\tau = u_0 + \tau R\left(u_0 + \frac{\tau}{2}R(u_0)\right) +$$

$$+ \tau A\left(u_0 + \tau R\left(u_0 + \frac{\tau}{2}R(u_0)\right) + \frac{\tau}{2}A\left(u_0 + \tau R\left(u_0 + \frac{\tau}{2}R(u_0)\right)\right)\right),$$

expanding the terms we get

$$\tilde{u}_\tau = u_0 + \tau R\left(u_0 + \frac{\tau}{2}R(u_0)\right) + \tau Au_0$$

$$+ \tau^2 AR\left(u_0 + \frac{\tau}{2}R(u_0)\right) + \frac{\tau^2}{2}A^2 u_0 + \frac{\tau^3}{2}A^2 R\left(u_0 + \frac{\tau}{2}R(u_0)\right).$$

We apply the Taylor-formula for R and also for $A \circ R$ with increment $\frac{\tau}{2}R(u_0)$, where $\left(A \circ R(x)\right)' = A'(R(x)) \circ R'(x) = AR'(x)$.

$$\tilde{u}_\tau = u_0 + \tau\left(R(u_0) + \frac{\tau}{2}R(u_0)R'(u_0)\right) + \tau Au_0 +$$

$$+ \tau^2 AR(u_0) + \tau^2 AR'(u_0)\frac{\tau}{2}R(u_0) + \frac{\tau^2}{2}A^2 u_0 + \varepsilon(\tau)\tau^2 =$$

$$= u_0 + \tau\left(R(u_0) + Au_0\right) + \frac{\tau^2}{2}\left(R(u_0)R'(u_0) + 2A\left(R(u_0)\right) + A^2 u_0\right) + \varepsilon(\tau)\tau^2.$$

The error becomes:

$$u_\tau - \tilde{u}_\tau = \left(R'(u_0)Au_0 - AR(u_0) \right)\frac{\tau^2}{2} + \varepsilon(\tau)\tau^2.$$

$\square$

As we can see this combined method is of first order although the applied numerical scheme ensures second order accuracy. The use of sequential splitting results in order reduction. We followed the same ideas and calculated the orders for combinations of the introduced splitting methods the SEQ, the SW and the MS splitting and four different numerical schemes. The explicit Euler, the improved Euler method which is of second order, the third order Heun and the fourth order Runge-Kutta method. The first order and the improved Euler method were defined, we give the algorithm for the Heun method applied on the autonomous equation $u'(t) = F(u(t))$:

$$\tilde{u}_\tau = u_0 + \frac{\tau}{4}F(u_0) + \frac{3\tau}{4}F\left(u_0 + \frac{2\tau}{3}F\left(u_0 + \frac{\tau}{3}F(u_0)\right)\right),$$

and the one for the Runge-Kutta method used here:

$$\tilde{u}_\tau = u_0 + \frac{\tau}{6}F(u_0) + \frac{\tau}{3}F\left(u_0 + \frac{\tau}{2}F(u_0)\right) + \frac{\tau}{3}F\left(u_0 + \frac{\tau}{2}F\left(u_0 + \frac{\tau}{2}F(u_0)\right)\right) +$$

$$+ \frac{\tau}{6}F\left(u_0 + \tau F\left(u_0 + \frac{\tau}{2}F\left(u_0 + \frac{\tau}{2}F(u_0)\right)\right)\right).$$

The table below contains our results on orders of different splittings coupled with different numerical methods. Symbolic calculations on for example MS splitting coupled with 4th order Runge-Kutta method becomes complicated. An algorithm was written in *Mathematica* for these symbolic calculations. The order of the

s	exp. Euler (1)	impr. Euler (2)	Heun (3)	Runge-Kutta (4)
SEQ (1)	1	1	1	1
SW (2)	1	2	2	2
MS (2)	1	2	2	2

Table 1: Local orders of combined methods for (4)

methods are in the parenthesis. A study of the order of combined methods for bounded linear problems can be found in [Csomós and Faragó]. Their results say that the order of the combined method is $s := \min\{p, r\}$, if p is the order of splitting and r denotes the order of the numerical method. The numbers of the above table are in accordance with their results.

4 The Fisher equation

The Fisher equation is:

$$\begin{cases} \partial_t u(t,x) & = & \partial_x^2 u(t,x) + u(t,x)(1 - u(t,x)) \qquad x \in \mathbb{R}, \ t \geqslant 0 \\ u(0,x) & = & \eta(x). \end{cases} \qquad (7)$$

There is only one chemical species present and one spatial variable here. This equation was originally derived to describe the propagation of a gene in a population [Fisher]. It is one of the simplest nonlinear models for reaction-diffusion equations. Such equations occur, e.g., in combustion, mass transfer, crystallization, plasma physics, and in general phase transition problems. See a discussion on reaction-diffusion models in [Érdi and Tóth] and [Murray]. For the initial condition:

$$u(0,x) = \frac{1}{(1 + k \exp(x/\sqrt{6}))^2}$$

wave form solution of the equation is known:

$$u(t,x) = \frac{1}{\left(1 + k \exp(-\frac{5}{6}t + \frac{1}{6}\sqrt{6}x)\right)^2}$$

and for:

$$u(0,x) = \frac{1}{(1 + k \exp(-x/\sqrt{6}))^2},$$

$$u(t,x) = \frac{1}{(1 + k \exp(-\frac{5}{6}t - \frac{1}{6}\sqrt{6}x))^2}$$

A natural way to split the Fisher equation is to decompose it into two subproblems: one for the diffusion and one that corresponds to the reaction part of the right hand side. Thus the definitions of the subproblems are:

$$\begin{cases} \partial_t u_1(t,x) = \partial_x^2 u_1(t,x) \\ u_1(0,x) \ = \eta_1(x) \end{cases} \qquad (8)$$

and

$$\begin{cases} \partial_t u_2(t,x) & = & u_2(t,x)(1 - u_2(t,x)) \\ u_2(0,x) & = & \eta_2(x), \end{cases} \qquad (9)$$

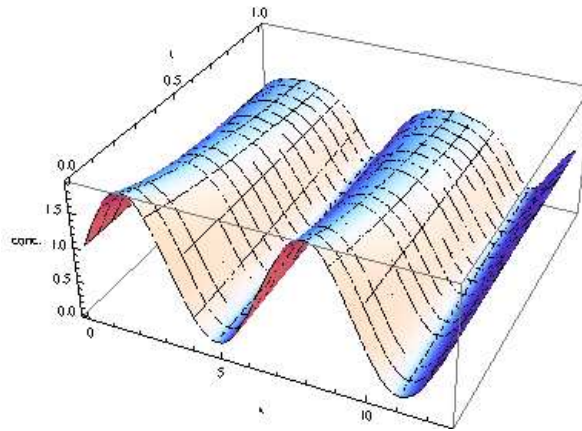where the initial condition $\eta_2(x) = u_1(\tau,x)$ connects the equations.

Figure 1: The exact solution of (9), $\eta_2(x) = \frac{9}{10}\sin(x) + 1$, $t \in [0,1]$ and $x \in [0,4\pi]$.

The exact solution of problem (9) is known, it is:

$$u_2(t,x) = \frac{\eta_2(x)e^t}{1 - \eta_2(x) + \eta_2(x)e^t}. \tag{10}$$

Since

$$\lim_{t \to \infty} u_2(t,x) = \begin{cases} 1 & \text{when} \quad \eta_2(x) \neq 0 \\ 0 & \text{when} \quad \eta_2(x) = 0 \end{cases}$$

the solution has two stationary states, namely: $u_2(t,x) \equiv 0$, $u_2(t,x) \equiv 1$. The $u_2(t,x) \equiv 1$ solution is asymptotically stable, whereas zero is an unstable equilibrium. Knowing the exact solution of this subproblem as a function of the initial condition means that we can symbolically solve this subproblem in each time step during the splitting procedure. It might be worth using the exact solution for comparisons in the study of the effect of splitting.

5   Numerical experiments

Here we introduce our numerical results on the Fisher equation. We solved both subproblems (8), (9) using the for numerical methods of different orders that were mentioned and considered in Section 3. We investigate the three splitting methods (SEQ, SW and MS). We calculated the errors and orders of the obtained combined methods numerically. Our test problem is the following initial–boundary value problem:

$$\begin{cases} \partial_t u(t,x) = \partial_x^2 u(t,x) + u(t,x)(1 - u(t,x)) \\ u(0,x) \quad = 1 + 0.9\sin(x) \\ u(t,0) \quad = 1 \\ u(t,4\pi) = 1 \end{cases} \quad , \qquad (11)$$

where $x \in [0, 4\pi]$ and $t \in [0, 1]$. We performed a spatial semidiscretization with
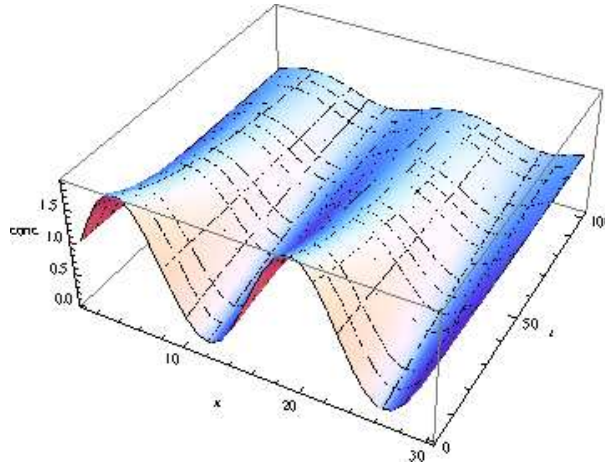

Figure 2: Reference solution generated by fourth order Runge-Kutta scheme, $\tau = 0.01$.

length parameter $\Delta x = \frac{4\pi}{30}$ that is we divided $[0, 4\pi]$ into 30 parts of equal length. Our tests showed that finer divisions provides no significantly more accurate solutions that is the obtained error is of the same magnitude as with 30. We approximated the spatial derivative with the well known second order scheme:

$$\partial_x^2 u(t,x_i) \approx \frac{u(t,x_{i+1}) - 2u(t,x_i) + u(t,x_{i-1}))}{\Delta x^2}.$$

After temporal discretization with $\tau = 0.01$ we solved the full problem (11) with the fourth order Runge-Kutta method. Taking a smaller time step resulted in solution that differs only in a magnitude of 10^{-6}. This is the reference solution for our study. In the experiments we used the same spatial division in every case, in fact we investigated the convergence of the semidiscrete submodels to the semidiscrete model: the reference solution. On the connection between the convergence to a semidiscrete model and convergence to a continuous model see [Larsson and Thomée].

5.1 Estimation of the local order of combined methods

We calculated the local error after the first time step that is at time τ with different time steps τ. We used the following values of τ:

τ_1	τ_2	τ_3	τ_4	τ_5	τ_6	τ_7	τ_8	τ_9	τ_{10}	τ_{11}
0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	0.1	0.11	0.12

Since the time step of the reference solution was 0.01 the evaluation of the error is simple. For a method with local order s the local error is:

$$e_{loc}(\tau) \approx c \cdot \tau^{s+1}$$

for small τ-s, where c is a constant which does not depend on τ. So for each i:

$$e_{loc}(\tau_i) \approx c \cdot \tau_i^{s+1}$$

and

$$\frac{e_{loc}(\tau_i)}{e_{loc}(\tau_{i+1})} \approx \left(\frac{\tau_i}{\tau_{i+1}} \right)^{s+1}$$

We can take the logarithm of both sides, then for each $i = 1, ..., 10$:

$$\frac{\log \frac{e_{loc}(\tau_i)}{e_{loc}(\tau_{i+1})}}{\log \frac{\tau_i}{\tau_{i+1}}} - 1 \approx s.$$

Evaluation of the left side shall give us the same value for every $i = 1, ..., 10$. We used *Mathematica*'s built–in procedures to fit a straight line of the form $y = ax$ on the dataset: $\left\{ \left(\log \frac{\tau_i}{\tau_{i+1}}, \log \frac{e_{loc}(\tau_i)}{e_{loc}(\tau_{i+1})} \right), i = 1, ..., 10 \right\}$. The following table contains the results of this calculation for different splittings and numerical methods. We

s	exp. Euler (1)	improved Euler (2)	Heun (3)	Runge-Kutta (4)
SEQ (1)	0.92	0.85	0.88	0.88
SW (2)	0.88	1.85	1.96	1.84
MS (2)	0.88	1.85	1.77	1.86

Table 2: Local order of combined methods for (11).

obtained values slightly closer to the expected ones by applying an extra additive parameter b in the fitted function of the form: $y = ax + b$. The parameter b varied

s	exp. Euler (1)	improved Euler (2)	Heun (3)	Runge-Kutta (4)
SEQ (1)	0.99	0.98	0.98	0.99
SW (2)	0.99	1.99	1.98	1.97
MS (2)	099.	1.99	1.90	1.98

Table 3: Estimated local order with additive parameter.

in the range $0.005 - 0.032$. We note that with the explicit Euler method increasing the order of splitting does not improve the results. The same pattern can be observed as in Section 3 namely that the local order of the combined method is the minimum of the local order of splitting and that of the numerical method.
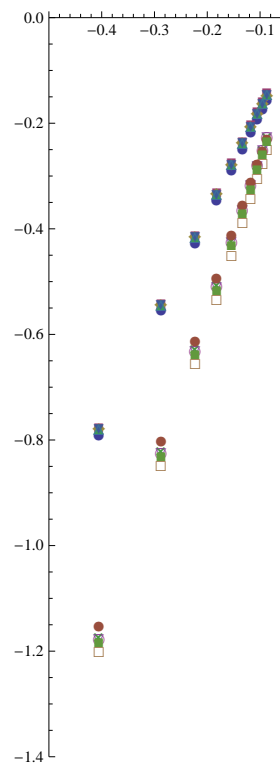

Figure 3: Local order estimations, for twelve different combined methods $\log \frac{e_{loc}(\tau_i)}{e_{loc}(\tau_{i+1})}$ against $\log \frac{\tau_i}{\tau_{i+1}}$ is plotted. Steepness of a fitted line gives the order of the method.

On figure 3 we can observe the two separate class of data: the one with steepness 2 that is with order 1, generated by using combined methods with SEQ or with explicit Euler method and the one with steepness 3, with order 2, generated by combined methods with SW or MS splitting combined with improved Euler, Heun or Runge-Kutta method.

5.2   Estimation of the global order

We evaluated the error at $T = 1$. We used time steps τ_i in such a way that we reach the end of the time interval $T = 1$ in a round number of steps.

τ_1	τ_2	τ_3	τ_4	τ_5	τ_6	τ_7
0.2	0.1	0.0625	0.05	0.04	0.025	0.02

As for the global error let us assume that it is of the form:

$$E(T, \tau_i) \approx C \cdot \tau_i^\rho \cdot T$$

for each $i = 1, ..., 7$, where C is a constant which does not depend on τ_i. In this case we can perform the same calculation as with the local error. Thus for each $i = 1, ..., 7$ we have:

$$\frac{\log \frac{E(T, \tau_i)}{E(T, \tau_{i+1})}}{\log \frac{\tau_i}{\tau_{i+1}}} \approx \rho.$$

Evaluation of the left side shall give us the same value for every $i = 1, ..., 7$. The following table contains the results of this calculation for different splittings and numerical methods. Since the solution of (9) is given in (10) as a function of the

ρ	exp. Euler	impr. Euler	Heun	Runge-Kutta
SEQ $(p = 1)$	1.04	0.99	1.08	1.08
SW $(p = 2)$	1.02	2.07	2.01	1.98
MS $(p = 2)$	1.02	2.07	1.95	1.998

Table 4: Estimation of orders of combined methods for (11).

initial condition we can use it in calculations instead of the numerical solution. The table below contains results generated by using (10) in each time step.

ρ $(h = \tau)$	$r = 1$	$r = 2$	$r = 3$	$r = 4$
SEQ $(p = 1)$	1.03	1.02	1.01	1.01
SW $(p = 2)$	1.01	2.06	1.95	1.98
MS $(p = 2)$	1.03.	2.00	1.99	1.99

Table 5: Estimation of orders of combined methods for (11), using (10).

6   Discussion and perspectives

We presented symbolic calculations for orders of ODE solving methods. Our motivation is to predict the order in the case when beside numerical procedures of certain order operator splitting is also used. We calculated the order of combined methods applied for systems of semilinear ODE-s like (4), where a bounded linear operator and a nonlinear operator is present. We presented numerical calculations on a test problem, the results are in accordance with our theoretical results. The results indicates that the combined method inherits the smaller one of the order of the splitting and the numerical method.

We intend to extend our investigations to methods where the numerical time step is different from the splitting time step. We plan to do numerical investigations on more realistic chemistry models, a system with two or three species and two spatial dimensions.

7   Acknowledgements

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(Received July 31, 2011)