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Abstract

In this paper we consider various multi-component splittings based on the trapezoidal rule and the implicit midpoint rule. It will be shown that an important requirement on such methods is internal stability. The methods will be applied to initial-boundary-value problems. Along with a theoretical analysis, some numerical test results will be presented.

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1. Introduction

In this paper we will discuss the accuracy and stability of some splitting methods which are based on the trapezoidal rule and implicit midpoint rule. The methods are used for the numerical solution of initial-boundary value problems for partial differential equations (PDEs) in two or three space dimensions with reaction and source terms. Discretization in space leads to large systems of ordinary differential equations (ODEs)

$$u'(t) = F(t, u(t)) \tag{1.1}$$

with $0 \leq t \leq T$ and given initial value $u(0)$. The function F contains the discretized spatial derivatives. We consider numerical schemes with step size τ yielding approximations u_n to the exact solution $u(t_n)$ at time levels $t_n = n\tau$ for $n = 0, 1, 2, \cdots$, starting with $u_0 = u(0)$.

Two standard methods are the trapezoidal rule

$$u_{n+1} = u_n + \tfrac{1}{2}\tau F(t_n, u_n) + \tfrac{1}{2}\tau F(t_{n+1}, u_{n+1}), \tag{1.2}$$

and the implicit midpoint rule

$$u_{n+1} = u_n + \tau F(t_{n+1/2},\ \tfrac{1}{2}u_n + \tfrac{1}{2}u_{n+1}). \tag{1.3}$$

The methods have order 2 and they are symmetric [4]. Both methods involve an implicit system with the whole function F. For discretized multi-dimensional PDEs the dimension of

the system will be very large and F may also contain different types of operations, such as convection-diffusion in various directions and nonlinear reaction terms, which makes it difficult to solve the implicit relations efficiently.

It is often possible to decompose the function F into a number of simpler component functions,

$$F(t,w) = F_1(t,w) + F_2(t,w) + \cdots + F_s(t,w). \tag{1.4}$$

Application of ODE methods to each individual component F_i can be much easier than to the whole F. We shall consider some splitting methods where in each stage only one of the components is treated implicitly. The best known method of this type is the ADI-Peaceman-Rachford method. This method, however, can only deal with 2-component splittings, see [14]. The related ADI method of Douglas is suited for arbitrary number of components, but it is no longer unconditionally stable for convection-diffusion problems if $s > 2$, see [8]. In this paper we restrict ourselves to second order methods that are unconditionally stable, in the von Neumann sense, for convection-diffusion problems for any value of s.

We consider the following method of Yanenko [16], based on a sequence of trapezoidal steps,

$$\begin{aligned} v_0 &= u_n, \\ v_i &= v_{i-1} + \tfrac{1}{2}\tau\Big(F_i(t_n + c_{i-1}\tau, v_{i-1}) + F_i(t_n + c_i\tau, v_i)\Big) \qquad (i = 1, 2, \cdots, s), \end{aligned} \tag{1.5}$$

with internal vectors v_i. If one stops here and accepts $u_{n+1} = v_s$ as the next approximation, the order of the method will only be 1, except for special situations with commuting operators. Order 2 of the method is obtained if the sequence of $F_1, F_2, \cdots, F_s$ is interchanged in the next step (Strang splitting). This gives, with $i = 1, 2, \cdots, s$,

$$\begin{aligned} v_{s+i} &= v_{s+i-1} + \tfrac{1}{2}\tau\Big(F_{s+1-i}(t_{n+2} - c_{s+1-i}\tau, v_{s+i-1}) + F_{s+1-i}(t_{n+2} - c_{s-i}\tau, v_{s+i})\Big) \\ u_{n+2} &= v_{2s}. \end{aligned} \tag{1.6}$$

We use the time levels $c_0 = 0, c_s = 1$. The other c_j are set to $1/2$, which is somewhat arbitrary (see Section 5). Irrespective of the choice, the method is symmetrical and of order 2. In the same way one can construct a method using the implicit midpoint rule in each of the fractional steps, which will lead to a method with very similar errors, see [7].

The two steps (1.5) and (1.6) should be considered together as one step, with step size 2τ, carrying u_n to u_{n+2} for $n = 0, 2, 4, \cdots$. We shall compare this method of Yanenko with two more simple methods where the fractional steps are performed by backward and forward Euler formulas with halved step size. Note that the trapezoidal method itself can be viewed as a forward Euler step followed by a backward Euler step with $\tau/2$ for the sub-steps. Likewise, the implicit midpoint rule consists of a backward Euler step followed by a forward Euler step.

The first method we propose is related, in the above sense, to the trapezoidal rule, and will therefore be called *trapezoidal splitting*, or, more formally, the trapezoidal splitting method. The method is given by

$$\begin{aligned} v_0 &= u_n, \\ v_i &= v_{i-1} + \tfrac{1}{2}\tau F_i(t_n, v_{i-1}) \qquad (i = 1, 2, \cdots, s), \\ v_{s+i} &= v_{s+i-1} + \tfrac{1}{2}\tau F_{s+1-i}(t_{n+1}, v_{s+i}) \qquad (i = 1, 2, \cdots, s), \\ u_{n+1} &= v_{2s}. \end{aligned} \tag{1.7}$$

Again, the vectors v_j $(1 \le j \le s)$ are internal quantities without physical relevance, except for v_s which is a consistent approximation to $u(t_{n+1/2})$. Note that if $s = 1$ the method reduces to the trapezoidal rule.

Similarly we can construct a splitting method based on the midpoint rule,

$$\begin{aligned} v_0 &= u_n, \\ v_i &= v_{i-1} + \tfrac{1}{2}\tau F_i(t_{n+1/2}, v_i) \qquad (i = 1, 2, \cdots, s), \\ v_{s+i} &= v_{s+i-1} + \tfrac{1}{2}\tau F_{s+1-i}(t_{n+1/2}, v_{s+i-1}) \qquad (i = 1, 2, \cdots, s), \\ u_{n+1} &= v_{2s}. \end{aligned} \tag{1.8}$$

We shall refer to (1.8) as the *midpoint splitting* method.

Both methods (1.7) and (1.8) have order two and they are symmetrical. If all F_j are linear, say $F_j(t, u) = A_j u$, with commuting matrices A_j, then the methods are identical, namely

$$u_{n+1} = \Big(\prod_{i=1}^{s}(I - \tfrac{1}{2}\tau A_i)\Big)^{-1}\Big(\prod_{i=1}^{s}(I + \tfrac{1}{2}\tau A_i)\Big)u_n. \tag{1.9}$$

Because of the close relation between the trapezoidal rule and midpoint rule, one would expect both splitting methods to behave similarly. As we shall see this is not so for semi-discrete PDE systems arising from initial-boundary value problems.

The above splitting methods (1.7), (1.8) seem not to have been studied in the literature. A linearized version of (1.7) was introduced in [1] for $s = 2$. Formula (1.9) can be found in [14], p.87, for $s = 3$, but a variety of very different methods can be based on this formula. Indeed, the following experiment shows a remarkable difference in behaviour between the midpoint and trapezoidal splitting methods.

Example 1.1. Consider the diffusion equation on domain $\Omega = (0, 1)^2$,

$$\begin{aligned} \mathbf{u}_t &= \mathbf{u}_{xx} + \mathbf{u}_{yy} + f(x, y, t) \qquad \text{on } \Omega, \\ \mathbf{u} &= 0 \qquad \text{on } \Gamma = \partial\Omega, \end{aligned}$$

with given initial value at $t = 0$ and source term f derived from the exact solution

$$\mathbf{u}(x, y, t) = e^t\, x(1 - x)y(1 - y)(16 + y).$$

The spatial derivatives are discretized with standard second order finite differences, and we make a dimensional splitting with $s = 2$ and equal distribution of the source term. So, $F_1(t, u)$ will be the finite difference approximation of $\mathbf{u}_{xx} + \frac{1}{2}f(t)$, and likewise for F_2 in the y-direction. Note that since the exact solution is a polynomial in x and y of degree ≤ 3, there will be no spatial error. The spatial grid has mesh width $h = 1/(m + 1)$ in both direction with m the number of grid points per direction. In Table 1.1 we have listed the errors, measured in the discrete L_2-norm, at the end time $T = 0.75$ for $h = 1/40$ with different values of the time step τ.

$1/\tau$	10	20	40	80
TrapSplit	$3.3\ 10^{-3}$	$8.3\ 10^{-4}$	$2.1\ 10^{-4}$	$5.2\ 10^{-5}$
MidpSplit	3.3	$8.5\ 10^{-1}$	$2.1\ 10^{-1}$	$5.3\ 10^{-2}$

Table 1.1. L_2-errors for $h = 1/40$ with trapezoidal splitting and midpoint splitting.

Clearly there is a huge difference between the two splitting methods. The difference becomes even more striking if the spatial mesh is refined, see Table 1.2. Although both methods have order two (in the classical ODE sense), the error constants for the midpoint splitting apparently contain negative powers of h.

$1/\tau$	10	20	40	80
TrapSplit	$3.4\ 10^{-3}$	$8.5\ 10^{-4}$	$2.1\ 10^{-4}$	$5.3\ 10^{-5}$
MidpSplit	9.2	2.3	$5.8\ 10^{-1}$	$1.5\ 10^{-1}$

Table 1.2. L_2-errors for $h = 1/80$ with trapezoidal splitting and midpoint splitting.

In this paper both methods will be analyzed to explain these numerical results. The method of Yanenko has been analyzed in [7] for $s = 2$ and in the paper of Čiegis and Kiškis [3] for arbitrary s. The analysis in the present paper follows the same approach. As we shall see the disappointing behaviour of the midpoint splitting in the above test is due to lack of so-called *internal stability*. Further it will be shown that the order of convergence for the trapezoidal splitting can be less than 2 upon simultaneous refinement of mesh width and time step if $s \geq 3$, but still the results are favourable compared to Yanenko's method.

This analysis is given in the Section 2, 3 and 4. In Section 5 boundary corrections are discussed. Section 6 contains numerical comparisons between the trapezoidal splitting method (1.7) and Yanenko's method (1.5),(1.6).

2. Internal perturbations

2.1. Preliminaries

The analysis will be performed for the linear case

$$F_j(t, w) = A_j w + g_j(t), \tag{2.1}$$

with $M \times M$ matrices A_j and $g_j(t) \in \mathbb{R}^M$. It is assumed that the problem represents a semi-discrete PDE, so the dimension depends on the mesh width in space h and some of the matrices A_j will contain negative powers of h. For inhomogeneous boundary conditions, the terms g_j will contain the boundary values relevant to A_j, which will also lead to negative powers of h, see for example [7, 9] for a more detailed description.

Results on stability and convergence will be obtained for the discrete L_2-norm on $\mathbb{R}^M$, $\|w\| = (M^{-1} w^T w)^{1/2}$, under the assumption

$$w^T A_j w \leq 0 \quad \text{for all} \quad w \in \mathbb{R}^M. \tag{2.2}$$

This implies that for any $\tau > 0$ we have

$$\|(I - \tfrac{1}{2}\tau A_j)^{-1}\| \leq 1, \qquad \|(I - \tfrac{1}{2}\tau A_j)^{-1}(I + \tfrac{1}{2}\tau A_j)\| \leq 1. \tag{2.3}$$

Note that (2.2) imposes no restriction on the norm $\|A_j\|$. So, the A_j may contain negative powers of h with arbitrary small $h > 0$. Further we will use the notations $Z_j = \tau A_j$ and $P_j = (I + \frac{1}{2}\tau A_j)$, $Q_j = (I - \frac{1}{2}\tau A_j)$.

2.2. Internal stability of trapezoidal splitting

Consider the trapezoidal splitting formula with perturbations $\rho_1, \cdots, \rho_{2s}$ on the stages,

$$\begin{aligned} \tilde{v}_0 &= \tilde{u}_n, \\ \tilde{v}_i &= \tilde{v}_{i-1} + \tfrac{1}{2}\tau F_i(t_n, \tilde{v}_{i-1}) + \rho_i \qquad (i = 1, 2, \cdots, s), \\ \tilde{v}_{s+i} &= \tilde{v}_{s+i-1} + \tfrac{1}{2}\tau F_{s+1-i}(t_{n+1}, \tilde{v}_{s+i}) + \rho_{s+i} \qquad (i = 1, 2, \cdots, s), \\ \tilde{u}_{n+1} &= \tilde{v}_{2s}. \end{aligned} \tag{2.4}$$

Let $e_n = \tilde{u}_n - u_n$. By subtracting (2.4) from (1.7) and eliminating the internal quantities $\tilde{v}_j - v_j$, it follows in a straightforward way that

$$e_{n+1} = R\, e_n + d_n \tag{2.5}$$

with stability matrix

$$R = Q_1^{-1} Q_2^{-1} \cdots Q_s^{-1} P_s \cdots P_2 P_1 \tag{2.6}$$

and with d_n containing the internal perturbations,

$$\begin{aligned} d_n &= Q_1^{-1} \cdots Q_s^{-1} \Big(P_s \cdots P_2 \rho_1 + P_s \cdots P_3 \rho_2 + \cdots + P_s \rho_{s-1} + \rho_s \Big) + \\ &\quad + Q_1^{-1} \cdots Q_s^{-1} \rho_{s+1} + Q_1^{-1} \cdots Q_{s-1}^{-1} \rho_{s+2} + \cdots + Q_1^{-1} \rho_{2s}. \end{aligned} \tag{2.7}$$

So, the matrix R determines how an error already present at time t_n will be propagated to t_{n+1}, whereas d_n stands for the local error introduced during the step. The usual step-by-step stability of the scheme is thus governed by R. Assuming that the matrices commute we have $\|R\| \leq 1$, so the method will be stable. Under this assumption it also follows that

$$\|d_n\| \leq \|\rho_1\| + \|\rho_2\| + \cdots + \|\rho_{2s}\|, \tag{2.8}$$

since any explicit factor P_j occurring in (2.7) is balanced by its implicit counterpart Q_j^{-1}. This means that the internal perturbations will not disrupt the result of a single step of the method. So, the method is *internally stable*, in the above sense.

2.3. Internal instability of midpoint splitting

For the midpoint splitting we can proceed similarly as in the preceding subsection. We consider along with (1.8) a perturbed version

$$\begin{aligned} \tilde{v}_0 &= \tilde{u}_n, \\ \tilde{v}_i &= \tilde{v}_{i-1} + \tfrac{1}{2}\tau F_i(t_{n+1/2}, \tilde{v}_i) + \rho_i \qquad (i = 1, 2, \cdots, s), \\ \tilde{v}_{s+i} &= \tilde{v}_{s+i-1} + \tfrac{1}{2}\tau F_{s+1-i}(t_{n+1/2}, \tilde{v}_{s+i-1}) + \rho_{s+i} \qquad (i = 1, 2, \cdots, s), \\ \tilde{u}_{n+1} &= \tilde{v}_{2s}. \end{aligned} \tag{2.9}$$

By eliminating the internal vectors $\tilde{v}_i - v_i$ it follows that the global errors $e_n = \tilde{u}_n - u_n$ satisfy

$$e_{n+1} = R\, e_n + d_n \tag{2.10}$$

with

$$R = P_1 P_2 \cdots P_s Q_s^{-1} \cdots Q_2^{-1} Q_1^{-1} \tag{2.11}$$

and with local errors d_n now given by

$$\begin{aligned} d_n &= P_1 \cdots P_s \Big(Q_s^{-1} \cdots Q_1^{-1} \rho_1 + Q_s^{-1} \cdots Q_2^{-1} \rho_2 + \cdots + Q_s^{-1} \rho_s \Big) + \\ &\quad + P_1 \cdots P_{s-1} \rho_{s+1} + P_1 \cdots P_{s-2} \rho_{s+2} + \cdots + P_1 \rho_{2s-1} + \rho_{2s}. \end{aligned} \tag{2.12}$$

Note that the stability matrix R has a similar structure as with the trapezoidal splitting. Again, if the matrices A_j commute then the assumption (2.2) implies $\|R\| \leq 1$. However, the propagation of the internal perturbations is now completely different. We only have a moderate propagation of ρ_1 and ρ_{2s}. For the other perturbation there are more explicit factors than implicit ones. With increasing stiffness, that is, if $h \to 0$, these explicit factors may introduce a blow-up of the local error d_n. So, the midpoint splitting is *not internally stable* for small h.

This lack of internal stability will necessitate a very accurate solution of the implicit relations in the internal stages to make the factors ρ_i small. As we shall see in the next section, the midpoint splitting seems unsuited for stiff ODEs anyway, since the local discretization errors are also not bounded uniformly in the mesh width h.

3. Local discretization errors

3.1. Local errors for trapezoidal splitting

The error bounds will be based on derivatives of the exact solution $u(t)$ and $\varphi_j(t) = F_j(t, u(t))$. If the PDE solution is smooth, we may assume that these derivatives are bounded uniformly in the mesh width h. Error bounds can also be derived directly in terms of the PDE solution by including the spatial errors in the derivation, see [15], but for simplicity we shall consider here the error with respect to the ODE solution.

In the following we shall use the notation $\mathcal{O}(\tau^p)$ to denote a vector or matrix whose L_2-norm is bounded by $C\tau^p$ with constant $C > 0$ independent of h. So, in particular, we do *not* have $A_j = \mathcal{O}(1)$ if A_j contains discretized spatial derivatives.

Suitable expressions for the local discretization errors can be easily derived by using the internal perturbations. Consider (2.4) with $\tilde{u}_n = u(t_n)$, so that $e_n = u(t_n) - u_n$ is the global discretization error. Hence, d_n is then the local discretization error, that is, the error introduced in one single step of the method. For the intermediate vectors $\tilde{v}_i$ we can take $\tilde{v}_i = u(t_n)(1 \leq i \leq s)$ and $\tilde{v}_{s+i} = u(t_{n+1})(1 \leq i \leq s)$. Note that the actual choice for these vectors is not important since we are only interested in the overall local error d_n, but with the above choice we get simple expressions for the residuals, namely

$$\begin{aligned} \rho_i &= -\tfrac{1}{2}\tau\varphi_i(t_n) \qquad (i = 1, \cdots, s), \\ \rho_{s+1} &= u(t_{n+1}) - u(t_n) - \tfrac{1}{2}\tau\varphi_s(t_{n+1}), \\ \rho_{s+i} &= -\tfrac{1}{2}\tau\varphi_{s+1-i}(t_{n+1}) \qquad (i = 2, \cdots, s). \end{aligned}$$

We shall elaborate the error for $s = 2$ and $s = 3$. Inserting the above residuals in (2.7), we obtain for $s = 3$

$$\begin{aligned} d_n &= (I - \tfrac{1}{2}Z_1)^{-1}(I - \tfrac{1}{2}Z_2)^{-1}(I - \tfrac{1}{2}Z_3)^{-1}\Big(-(I + \tfrac{1}{2}Z_3)(I + \tfrac{1}{2}Z_2)\tfrac{1}{2}\tau\varphi_1(t_n) - \\ &\quad -(I + \tfrac{1}{2}Z_3)\tfrac{1}{2}\tau\varphi_2(t_n) - \tfrac{1}{2}\tau\varphi_3(t_n) + u(t_{n+1}) - u(t_n) - \tfrac{1}{2}\tau\varphi_3(t_{n+1}) - \\ &\quad -(I - \tfrac{1}{2}Z_3)\tfrac{1}{2}\tau\varphi_2(t_{n+1}) - (I - \tfrac{1}{2}Z_3)(I - \tfrac{1}{2}Z_2)\tfrac{1}{2}\tau\varphi_1(t_{n+1})\Big). \end{aligned}$$

Using

$$u(t_{n+1}) - u(t_n) = \tfrac{1}{2}\tau\Big(F(t_n, u(t_n)) + F(t_{n+1}, u(t_{n+1}))\Big) - \tfrac{1}{12}\tau^3 u'''(t_{n+1/2}) + \cdots,$$

it follows by some calculations that

$$\begin{aligned} d_n \quad &= (I - \tfrac{1}{2}Z_1)^{-1}(I - \tfrac{1}{2}Z_2)^{-1}(I - \tfrac{1}{2}Z_3)^{-1}\Big(-\tfrac{1}{4}\tau Z_3 Z_2 \varphi_1(t_{n+1/2}) + \\ &\quad + \tfrac{1}{4}\tau^2(Z_2 + Z_3)\varphi_1'(t_{n+1/2}) + \tfrac{1}{4}\tau^2 Z_3 \varphi_2'(t_{n+1/2})\Big) + \mathcal{O}(\tau^3). \end{aligned} \tag{3.1}$$

The corresponding formula for $s = 2$ simply follows from this by setting $Z_3 = 0, \varphi_3 = 0$. So, for $s = 2$ the local discretization error is

$$d_n = (I - \tfrac{1}{2}Z_1)^{-1}(I - \tfrac{1}{2}Z_2)^{-1}\tfrac{1}{4}\tau^2 Z_2 \varphi_1'(t_{n+1/2}) + \mathcal{O}(\tau^3). \tag{3.2}$$

Using (2.3) it follows directly from (3.2) that $d_n = \mathcal{O}(\tau^2)$. Note that for fixed h we get an $\mathcal{O}(\tau^3)$ bound due to the hidden τ in Z_2. To obtain a similar bound uniformly in h, we need the compatibility condition $A_2\varphi_1(t) = \mathcal{O}(1)$. This condition will only be satisfied in special cases, namely where $\varphi_1(t)$ satisfies homogeneous boundary conditions relevant to A_2. It should be noted that also fractional order results are possible: if $A_2^\alpha \varphi_1(t) = \mathcal{O}(1)$ with $\alpha \in (0, 1)$, it can be shown that $d_n = \mathcal{O}(\tau^{2+\alpha})$.

For the formula with $s = 3$ similar considerations hold. To guarantee that $d_n = \mathcal{O}(\tau^3)$ we now get several compatibility conditions. If we assume only that A_2 and A_3 commute, it follows from (2.3) only that $d_n = \mathcal{O}(\tau)$, which is a poor result of course since this is the error introduced in a single step.

We note that, assuming smoothness of the exact solution, compatibility conditions like $A_2\varphi_1(t) = \mathcal{O}(1)$ will certainly hold if there are no boundary conditions present, for example with periodicity conditions. So, any deviation from the classical ODE results is here entirely due to boundary conditions.

In the next section we shall present some convergence results for initial-boundary value problems where the compatibility conditions need not hold.

3.2. Local errors for midpoint splitting

In the same way we can derive an expression for the local discretization errors of the midpoint splitting. We take $\tilde{v}_0 = u(t_n), \tilde{v}_{2s} = u(t_{n+1})$ and $\tilde{v}_j = u(t_{n+1/2})$ for the other j. This gives residuals

$$\begin{aligned} \rho_1 \quad &= u(t_{n+1/2}) - u(t_n) - \tfrac{1}{2}\tau\varphi_1(t_{n+1/2}), \\ \rho_i \quad &= -\tfrac{1}{2}\tau\varphi_i(t_{n+1/2}) \qquad (i = 2, \cdots, s), \\ \rho_{s+i} \quad &= -\tfrac{1}{2}\tau\varphi_{s+1-i}(t_{n+1/2}) \qquad (i = 1, \cdots, s-1), \\ \rho_{2s} \quad &= u(t_{n+1}) - u(t_{n+1/2}) - \tfrac{1}{2}\tau\varphi_1(t_{n+1/2}). \end{aligned}$$

We elaborate the local error for $s = 2$ only. Since the result will be negative it is not necessary to consider larger values of s. For $s = 2$ we obtain $\rho_2 = \rho_3 = -\tfrac{1}{2}\tau\varphi_2(t_{n+1/2})$ and

$$\begin{aligned} \rho_1 \quad &= \tfrac{1}{2}\tau\varphi_2(t_{n+1/2}) - \tfrac{1}{8}\tau^2 u''(t_{n+1/2}) + \mathcal{O}(\tau^3), \\ \rho_4 \quad &= \tfrac{1}{2}\tau\varphi_2(t_{n+1/2}) + \tfrac{1}{8}\tau^2 u''(t_{n+1/2}) + \mathcal{O}(\tau^3). \end{aligned}$$

After some calculations it follows that

$$d_n = (R-I)\Big(\tfrac{1}{4}\tau Z_1\varphi_2(t_{n+1/2}) - \tfrac{1}{8}\tau^2 u''(t_{n+1/2})\Big) + \mathcal{O}(\tau^3). \tag{3.3}$$

In general, the factor with $Z_1\varphi_2$ contains negative powers of h, and these are not countered by $R-I$, which is $\mathcal{O}(1)$ only, not smaller. So, we can expect a growth of the temporal local discretization error if the mesh width h is decreased. The global discretization error then will show a similar unpleasant behaviour. This is precisely what was observed in the numerical results of Table 1.1 and 1.2.

Already we can conclude that the midpoint splitting, in its present form, is not suited for PDE problems with boundary conditions. Also with boundary corrections, see Section 5, this method seems not competitive with the trapezoidal splitting.

4. Global discretization errors

4.1. Error bounds for trapezoidal splitting

In this section convergence results will be derived for the trapezoidal splitting with $s = 2$ and $s = 3$. At the end of the section a comparison will be made with known results for the method of Yanenko (1.5),(1.6).

Throughout this section it will be assumed that the trapezoidal splitting is stable,

$$\|R^n\| \le C \qquad \text{for all} \quad n \ge 1 \tag{4.1}$$

with a constant $C = \mathcal{O}(1)$. As mentioned already in Section 3, this certainly holds if the matrices A_j commute and satisfy (2.2). Under this assumption one can prove convergence by bounding the local errors. However these local error bounds often give too pessimistic results, see for example [2, 10] for Runge-Kutta methods and [3, 7, 9] for splitting methods. We shall use the error decomposition as in [7],

$$d_n = (R-I)\xi_n + \eta_n \quad \text{with} \quad \xi_n = \mathcal{O}(\tau^p),\ \eta_n = \mathcal{O}(\tau^{p+1}),\ \xi_{n+1} - \xi_n = \mathcal{O}(\tau^{p+1}). \tag{4.2}$$

It is easy to show that this implies $e_n = \mathcal{O}(\tau^p)$ by writing out the global error in full before bounding the various contributions. Note that (4.2) implies $d_n = \mathcal{O}(\tau^p)$ only, and the fact that we have the same order for the global error e_n is a super-convergence phenomenon. This local error decomposition is only interesting for stiff equations; for fixed h we would have $R - I = \mathcal{O}(\tau)$, in which case (4.2) gives $d_n = \mathcal{O}(\tau^{p+1})$.

In the following we use the notation $A = A_1 + A_2 + \cdots + A_s$.

Theorem 4.1. Consider the trapezoidal splitting with $s = 2$, and assume that

$$A^{-1}A_2\varphi_1^{(k)}(t) = \mathcal{O}(1) \tag{4.3}$$

for $k = 1, 2$ and $t \in [0, T]$. Then the global discretization errors satisfy $e_n = \mathcal{O}(\tau^2)$ for $t_n \in [0, T]$.

Proof. We have

$$R - I = (I - \tfrac{1}{2}Z_1)^{-1}(I - \tfrac{1}{2}Z_2)^{-1}\Big(Z_1 + Z_2\Big).$$

Hence the local error (3.2) can be written as

$$d_n = (R - I)A^{-1}A_2 \tfrac{1}{4}\tau^2\varphi_1'(t_{n+1/2}) + \mathcal{O}(\tau^3).$$

Clearly this fits into the form (4.2) with $\xi_n = \frac{1}{4}\tau^2 A^{-1}A_2\varphi_1'(t_{n+1/2})$, and thus we obtain the second order convergence result. □

Note that the above result also holds for noncommuting A_1 and A_2. However, to verify the underlying assumptions it is helpful to assume that the matrices do commute. It is easy to show that if A_1 and A_2 are negative definite and commuting, then $A^{-1}A_2 = \mathcal{O}(1)$.

It is obvious from the proof that the assumption in the theorem could be formulated a bit more general. What we need is only the existence of a function v, with $v(t), v'(t) = \mathcal{O}(1)$, satisfying $Av(t) = A_2\varphi_1'(t)$ for all t. This would allow A to be singular. The following results permit a similar generalization.

Theorem 4.2. Consider the trapezoidal splitting with $s = 3$ and let $M = A + \frac{1}{4}\tau^2 A_3A_2A_1$. If it holds that

$$\tau M^{-1}A_3A_2\varphi_1^{(k)}(t) = \mathcal{O}(1) \tag{4.4}$$

for $k = 0, 1$ and $t \in [0, T]$, then $e_n = \mathcal{O}(\tau)$ for $t_n \in [0, T]$. Under the stronger condition

$$M^{-1}\Big(A_3A_2\varphi_1^{(k)}(t) - (A_2 + A_3)\varphi_1^{(k+1)}(t) - A_3\varphi_2^{(k+1)}(t)\Big) = \mathcal{O}(1) \tag{4.5}$$

for $k = 0, 1$ and $t \in [0, T]$, we have $e_n = \mathcal{O}(\tau^2)$ for $t_n \in [0, T]$.

Proof. For $s = 3$ we have

$$R - I = (I - \tfrac{1}{2}Z_1)^{-1}(I - \tfrac{1}{2}Z_2)^{-1}(I - \tfrac{1}{2}Z_3)^{-1}\Big((Z_1 + Z_2 + Z_3) + \tfrac{1}{4}Z_3Z_2Z_1\Big).$$

By using (3.1), the results follow in the same way as in the previous theorem. □

Corollary 4.3. Suppose the matrices A_j are negative definite and commuting. If either $A_2 = \mathcal{O}(1)$ or $A_3 = \mathcal{O}(1)$, then $e_n = \mathcal{O}(\tau^2)$ for $t_n \in [0, T]$.

Proof. If the A_j are commuting and negative definite, then

$$(A + \tfrac{1}{4}\tau^2 A_3A_2A_1)^{-1}A_j = \mathcal{O}(1),$$

and using $A_i = \mathcal{O}(1)$ for $i = 2$ or 3, it follows that (4.5) is satisfied. □

Corollary 4.4. Let $\alpha \in (0, \frac{1}{2})$, $\beta \geq 0$ with $2 - 4\alpha \leq \beta$. Suppose the matrices A_j are commuting and negative definite. Suppose in addition that $h^2A_j = \mathcal{O}(1)$, $A_3^\alpha A_2^\alpha\varphi_1(t) = \mathcal{O}(1)$ and $\tau h^{-\beta} = \mathcal{O}(1)$. Then $e_n = \mathcal{O}(\tau)$ for $t_n \in [0, T]$.

Proof. If the A_j are commuting and negative definite the expression in (4.4) can be written as

$$[\tau A_3^{(1/2)-\alpha}A_2^{(1/2)-\alpha}]\,[(A + \tfrac{1}{4}\tau^2 A_3A_2A_1)^{-1}A_3^{1/2}A_2^{1/2}]\,[A_3^\alpha A_2^\alpha\varphi_1(t)],$$

and $(A + \frac{1}{4}\tau^2 A_3A_2A_1)^{-1}A_3^{1/2}A_2^{1/2} = \mathcal{O}(1)$. Using $2 - 4\alpha \leq \beta$, $h^2A_j = \mathcal{O}(1)$ and $\tau h^{-\beta} = \mathcal{O}(1)$, it follows that $\tau A_3^{(1/2)-\alpha}A_2^{(1/2)-\alpha} = \mathcal{O}(1)$, and thus (4.4) will hold. □

We note that the last corollary is relevant to parabolic equations. For the heat equation with Dirichlet boundary conditions we can apply this result with arbitrary $\alpha < 1/4$, see [2] or [9], for instance. An application will be given in Section 6.

4.2. Remarks on related results

A convergence result for the ADI-Peaceman-Rachford method has been presented in [9] for $s = 2$, showing also second order convergence under the assumption (4.3). It is somewhat surprising that the same result is valid for the trapezoidal splitting since the internal vectors v_j are not fully consistent.

For Yanenko's method (1.5),(1.6) applied to the s-dimensional heat equation, a similar analysis has been presented in [7] for $s = 2$ and in [3] for arbitrary s. The results are less favourable than for the trapezoidal splitting. Even for the simple 2-dimensional heat equation with homogeneous Dirichlet conditions, constant source term and $\tau/h = \mathcal{O}(1)$ we will have only $e_n = \mathcal{O}(\tau^{1/2})$ [3, 7], and the order of convergence 1/2 is also valid for $s \geq 3$ [3]. In Section 6 we shall give some numerical comparisons between (1.5),(1.6) and the trapezoidal splitting (1.7).

The order reduction due to boundary conditions can also be observed for Runge-Kutta methods, see Brenner et al. [2] for instance. In a recent paper, Lubich and Ostermann [12] have shown that for strongly A-stable Runge-Kutta methods, applied to parabolic equations, the classical order of convergence holds in the interior of the spatial domain. In some numerical tests on parabolic problems we observed that the same seems to hold for the trapezoidal splitting and Yanenko's method, in spite of the fact that these methods are not strongly stable for very stiff eigenvalues.

5. Boundary corrections

The fact that the splitting methods, which are second order in the classical ODE sense, do not always give second order convergence uniformly in h is due to the boundary conditions, see Section 3. One may therefore hope that this order reduction will disappear if we treat the boundaries as much as possible in the same way as the interior region. The formulas in Mitchell and Griffiths [14], Sections 2.12, 2.16, and LeVeque [11] are all constructed along this principle.

Boundary corrections can be derived for rectangular regions Ω. Assume for the moment that Dirichlet conditions are given on the whole boundary Γ. Let Γ_i be that part of the boundary on which the values are relevant to F_i, and let $\Gamma_{j,\ldots,k} = \bigcup_{i=j}^{k} \Gamma_i$, for $j < k$. If F_i contains no discretized spatial derivatives, then Γ_i is empty. In case F_i does contain spatial derivatives we can apply F_i on Γ_j for $j \neq i$, but not on Γ_i itself.

Due to its simple form it is easy to derive boundary corrections for the trapezoidal splitting. We note that $v_0 = u_n$ and $v_{2s} = u_{n+1}$ are consistent approximations to the exact solution u. Further, in (1.7) we need the value of v_{i-1} on Γ_i $(i = 1, \cdots, s)$, whereas v_{s+i} must be known on Γ_{s+1-i} $(i = 1, \cdots, s)$. For the corrected boundary conditions of the trapezoidal splitting we take $v_0 = u(t_n)$ on Γ, and subsequently

$$v_i = v_{i-1} + \tfrac{1}{2}\tau F_i(t_n, v_{i-1}) \quad \text{on} \quad \Gamma_{i+1,\ldots,s} \tag{5.1}$$

for $i = 1, 2, \cdots, s-1$, and likewise $v_{2s} = u(t_{n+1})$ on Γ,

$$v_{2s-j} = v_{2s+1-j} - \tfrac{1}{2}\tau F_j(t_{n+1}, v_{2s+1-j}) \quad \text{on} \quad \Gamma_{j+1,\ldots,s} \tag{5.2}$$

for $j = 1, 2, \cdots, s-1$.

With von Neumann boundary conditions the formulas (5.1) and (5.2) should be used to prescribe the outward normal derivatives of v_i and v_{s+i}, similar as in [11].

A natural way to derive boundary corrections for the midpoint splitting is to set $v_s = u(t_{n+1/2})$ on Γ, and then use (1.8) on the boundary to obtain

$$v_{s\pm i} = v_{s\pm(i-1)} \pm F_{s+1-i}(t_{n+1/2}, v_{s\pm(i-1)}) \quad \text{on} \quad \Gamma_{1,\ldots,i-1} \tag{5.3}$$

for $i = 1, 2, \cdots, s-1$. In some numerical tests the results of the midpoint splitting method showed considerable improvement with these boundary corrections, but still the midpoint splitting was not competitive with the trapezoidal splitting, due to its lack of internal stability. Therefore, we shall no longer consider this method. (It should be noted, however, that the midpoint splitting method did perform well in the test report [5], where the underlying decomposition of F was based on a Hopscotch type splitting and the PDE problem was advection dominated in two directions with a nonstiff reaction term.)

For Yanenko's method the situation is more complicated, due to the fact that v_i can not be written explicitly in terms of of either v_{i-1} or v_{i+1}, and the values of v_i are now needed on both Γ_i and Γ_{i+1} $(i = 1, 2, \cdots, s-1)$ for the step (1.5). For (1.6) this is similar, of course. Consider, for example, the first stage in (1.5), where v_1 is implicitly defined in terms of v_0. Starting with $v_0 = u(t_n)$ on Γ, we can approximate the implicit relation by

$$v_1 \approx u(t_n) + \tau F_1(t_n, u(t_n)).$$

However, since F_1 cannot be applied on Γ_1, in general, we can use this formula only on Γ_2 in the second stage of the method. As we have $F_1(t, u(t)) = u'(t) - \sum_{j=2}^{s} F_j(t, u(t))$, we can also take the approximate formula

$$v_1 \approx u(t_{n+1}) - \tau \sum_{j=2}^{s} F_j(t_{n+1}, u(t_{n+1})),$$

which now can be used on Γ_1. For the other v_j we can proceed similarly. This gives for the v_i $(i = 1, 2, \cdots, s-1)$ in (1.5) the formulas

$$\begin{aligned} v_i &= u(t_n) + \tau \sum_{j=1}^{i} F_j(t_n, u(t_n)) \quad \text{on} \quad \Gamma_{i+1}, \\ v_i &= u(t_{n+1}) - \tau \sum_{j=i+1}^{s} F_j(t_{n+1}, u(t_{n+1})) \quad \text{on} \quad \Gamma_i. \end{aligned} \tag{5.4}$$

Likewise for the v_{s+i} $(i = 1, 2, \cdots, s-1)$ in (1.6) we take

$$\begin{aligned} v_{s+i} &= u(t_{n+1}) + \tau \sum_{j=s+1-i}^{s} F_j(t_{n+1}, u(t_{n+1})) \quad \text{on} \quad \Gamma_{s-i}, \\ v_{s+i} &= u(t_{n+2}) - \tau \sum_{j=1}^{s-i} F_j(t_{n+2}, u(t_{n+2})) \quad \text{on} \quad \Gamma_{s+1-i}. \end{aligned} \tag{5.5}$$

Numerical results in [11] indicate that a better accuracy may be obtained if in (5.4),(5.5) higher order terms of τ are included to give a better approximation of the implicit relations. However, if $s > 2$ or nonlinear terms are involved, this leads to rather complicated correction terms.

We have not attempted to perform a detailed error analysis for the above boundary corrections along the lines of the previous section. Instead, we shall present in the next section several numerical results.

6. Numerical comparisons

In this section some numerical results are presented for Yanenko's method (1.5),(1.6) and the trapezoidal splitting method (1.7). Note that the computational work is almost identical for both methods. The measured error is the difference between the numerical results and the exact PDE solution, that is, the restriction of $\mathbf{u}$ to the grid. This includes also spatial errors, but it has been verified that the temporal errors are dominant in the following tables.

Example 6.1. We consider the 2-dimensional diffusion-reaction equation on spatial domain $\Omega = [0, 10]^2$ and $t \in [0, 10]$,

$$\mathbf{u}_t = \mathbf{u}_{xx} + \mathbf{u}_{yy} + \mathbf{u}^2(1 - \mathbf{u}) \qquad \text{on } \Omega,$$

with initial condition and Dirichlet boundary conditions chosen such that we have the exact solution

$$\mathbf{u}(x, y, t) = \Big(1 + \exp(\tfrac{1}{2}(x + y - t))\Big)^{-1}.$$

This solution consists of a wave traveling diagonally over the domain. The spatial derivatives are discretized with standard second order finite differences. Let $\delta_x^2(t)$ stand for the finite difference operator approximating $\mathbf{u}_{xx}$ with the associated time-dependent boundary conditions for $x = 0$ and $x = 10$. Likewise $\delta_y^2(t)$ approximates $\mathbf{u}_{yy}$ with boundary conditions at $y = 0$, $y = 10$. We consider the following splitting with $s = 3$,

$$F_1(t, w) = [\delta_x^2(t)]\, w, \quad F_2(t, w) = [\delta_y^2(t)]\, w, \quad F_3(t, w) = w^2(1 - w). \tag{6.1}$$

The multiplications in F_3 are to be interpreted componentwise. The spatial grid has mesh width h in both directions. In Table 6.1 the errors in L_2-norm are listed at time $T = 10$ with $\tau = h = 10/N$. Table 6.2 contains the same errors for the schemes with boundary corrections according to the formulas of Section 5.

N	10	20	40	80
Yanenko	$1.5\ 10^{-2}$	$6.9\ 10^{-3}$	$4.1\ 10^{-3}$	$2.7\ 10^{-3}$
TrapSplit	$3.8\ 10^{-3}$	$9.9\ 10^{-4}$	$2.5\ 10^{-4}$	$6.3\ 10^{-5}$

Table 6.1. Splitting (6.1). L_2-errors for Yanenko's method and trapezoidal splitting, no boundary corrections.

N	10	20	40	80
Yanenko	$1.1\ 10^{-2}$	$2.9\ 10^{-3}$	$7.4\ 10^{-4}$	$1.8\ 10^{-4}$
TrapSplit	$3.2\ 10^{-3}$	$8.2\ 10^{-4}$	$2.0\ 10^{-4}$	$5.1\ 10^{-5}$

Table 6.2. Splitting (6.1). L_2-errors for Yanenko's method and trapezoidal splitting, with boundary corrections.

In this example the trapezoidal splitting gives second order accuracy without boundary corrections. Although the assumptions of Corollary 4.3 are not fulfilled, the result seems to

apply here since $A_3 = \mathcal{O}(1)$, where A_3 is the Jacobi matrix associated with the reaction term F_3. Yanenko's method gives a low order of convergence without boundary corrections, also in agreement with the theoretical results for the linear case [7, 3]. With boundary corrections the second order is restored, but still the results are less accurate than for the trapezoidal splitting.

Example 6.2. We consider the same problem as in Example 6.1, but now with the splitting

$$F_1(t,w) = w^2(1-w), \quad F_2(t,w) = [\delta_x^2(t)]\, w, \quad F_3(t,w) = [\delta_y^2(t)]\, w. \tag{6.2}$$

Here we cannot expect second order convergence for the trapezoidal splitting since both A_2 and A_3 are not $\mathcal{O}(1)$. The errors are listed in the Tables 6.3 and 6.4 (with boundary corrections). Again the errors are measured in the L_2-norm at $T = 10$ with $\tau = h = 10/N$.

N	10	20	40	80
Yanenko	$1.4\ 10^{-2}$	$7.1\ 10^{-3}$	$4.2\ 10^{-3}$	$2.8\ 10^{-3}$
TrapSplit	$6.3\ 10^{-3}$	$1.8\ 10^{-3}$	$5.9\ 10^{-4}$	$2.3\ 10^{-4}$

Table 6.3. Splitting (6.2). L_2-errors for Yanenko's method and trapezoidal splitting, no boundary corrections.

N	10	20	40	80
Yanenko	$5.7\ 10^{-3}$	$1.6\ 10^{-3}$	$4.1\ 10^{-4}$	$1.1\ 10^{-4}$
TrapSplit	$2.1\ 10^{-3}$	$4.9\ 10^{-4}$	$1.2\ 10^{-4}$	$2.8\ 10^{-5}$

Table 6.4. Splitting (6.2). L_2-errors for Yanenko's method and trapezoidal splitting, with boundary corrections.

We see that here boundary corrections are also needed for the trapezoidal splitting to obtain second order accuracy. Without these corrections a first order convergence could be expected from Corollary 4.4. The actual order of convergence seems slightly better in Table 6.3, but tests with smaller τ and h did show an order of convergence close to one.

As in the previous example the results for the trapezoidal splitting are more favourable than for Yanenko's method.

Example 6.3. In this final example we consider advection coupled with a (mildly) stiff reaction term, on domain $\Omega = [0,1]^2$ and $t \in [0,1]$,

$$\mathbf{u}_t = a\mathbf{u}_x + b\mathbf{u}_y + f(\mathbf{u}) \qquad \text{on } \Omega,$$

with given velocities $a(x,y,t) = 2\pi(y - \frac{1}{2})$, $b(x,y,t)) = 2\pi(\frac{1}{2} - x)$, and with

$$\mathbf{u}(x,y,t) = \begin{pmatrix} \mathbf{u}_1(x,y,t) \\ \mathbf{u}_2(x,y,t) \end{pmatrix}, \qquad f(\mathbf{u}) = \begin{pmatrix} -k_1\mathbf{u}_1 + k_2\mathbf{u}_1\mathbf{u}_2 \\ k_1\mathbf{u}_1 - k_2\mathbf{u}_1\mathbf{u}_2 \end{pmatrix}.$$

The reaction constants are chosen as $k_1 = k_2 = 100$. Dirichlet conditions are given at the inflow boundaries. At the outflow boundaries we shall use an upwind discretization in space,

in the interior second order central differences are used. The spatial operators are now no longer negative definite, there will be eigenvalues close to the imaginary axis.

The velocity field will give a rotation around the center $(\frac{1}{2}, \frac{1}{2})$ of the domain. The exact solution can be found by superposition of this rotation upon the solution of the ODE system $v'(t) = f(v(t))$. To solve this ODE, note that we will have $v_1(t) + v_2(t) = d$, constant in time. By eliminating v_2 it follows that

$$v_1' = c\, v_1 - k_2\, v_1^2,$$

with $c = d\, k_2 - k_1$, and the exact solution is given by

$$v_1(t) = \frac{c\, v_1(0) \exp(c\, t)}{c + k_2\, v_1(0)(\exp(c\, t) - 1)}\,, \qquad v_2(t) = d - v_1(t).$$

For the PDE we take the initial value

$$\mathbf{u}_1(x, y, 0) = \tfrac{8}{10} + \tfrac{4}{10} \exp(-10(x - \tfrac{1}{2})^2 - 10(y - \tfrac{3}{4})^2), \qquad \mathbf{u}_2(x, y, 0) = 0.$$

In the rotating coordinate system

$$\xi = \cos(2\pi t)(x - \tfrac{1}{2}) - \sin(2\pi t)(y - \tfrac{1}{2}), \quad \eta = \sin(2\pi t)(x - \tfrac{1}{2}) + \cos(2\pi t)(y - \tfrac{1}{2}),$$

we define

$$d = d(x, y, t) = \tfrac{8}{10} + \tfrac{4}{10} \exp(-10\xi^2 - 10(\eta - \tfrac{1}{4})^2), \quad c = c(x, y, t) = d(x, y, t)k_1 - k_2,$$

giving the solution

$$\mathbf{u}_1(x, y, t) = \frac{c\, d\, \exp(c\, t)}{c + k_2\, d\, (\exp(c\, t) - 1)}\,, \qquad \mathbf{u}_2(x, y, t) = d - \mathbf{u}_1(x, y, t). \tag{6.3}$$

An illustration of this solution is shown in Figure 1.

Since the reaction term in this problem introduces a strong transient phase, we use an increasing step size sequence with small step sizes at the beginning. If the initial step size is too large the Newton process for the reaction term diverges. We have have chosen a ratio $\kappa = 20$ between the first and last step size. If N is the number of steps, then $\theta = \sqrt[N]{\kappa}$, $\tau_0 = (1 - 1/\theta)/(\kappa - 1)$ and $\tau_j = \tau_0 \theta^j$ for $j = 1, 2, ..., N$. For Yanenko's method we used a modification such that the step sizes in (1.5) and (1.6) are equal, namely, the above procedure was applied with N replaced by $N/2$ and the resulting step sizes were used to go from t_n to t_{n+2}. Also with these increasing step sizes we found divergence for both methods in the very first step with $N = 10$, so the following results are with $N \geq 20$.

We consider splitting with $F_1 \approx x$-advection, $F_2 \approx y$-advection and F_3 for the reaction term. The L_2-errors at time $T = 1$ are listed in Table 6.5.

N	20	40	80	160
Yanenko	$3.0\ 10^{-2}$	$1.4\ 10^{-2}$	$5.1\ 10^{-3}$	$1.8\ 10^{-3}$
TrapSplit	$3.0\ 10^{-2}$	$1.3\ 10^{-2}$	$4.8\ 10^{-3}$	$1.7\ 10^{-3}$

Table 6.5. Advection-reaction equation. L_2-errors for Yanenko's method and trapezoidal splitting, no boundary corrections.

Both methods give very similar results with an order of convergence approximately 3/2. We also tested the trapezoidal splitting with boundary corrections at the inflow boundaries, but, to our surprise, this gave nearly identical results. Finally, we tested the trapezoidal splitting with F_1 being the reaction term and with F_2, F_3 approximating the advection in x and y direction, respectively. Also this gave nearly identical results.

At the moment we do not have a theoretical explanation for these results, not even a heuristic one as in the two preceding examples. A more detailed analysis of the local error (3.1) seems to be needed for this specific example. The fact that boundary corrections did not give an improvement of the results indicates that the stiffness of the reaction term is an important factor here.

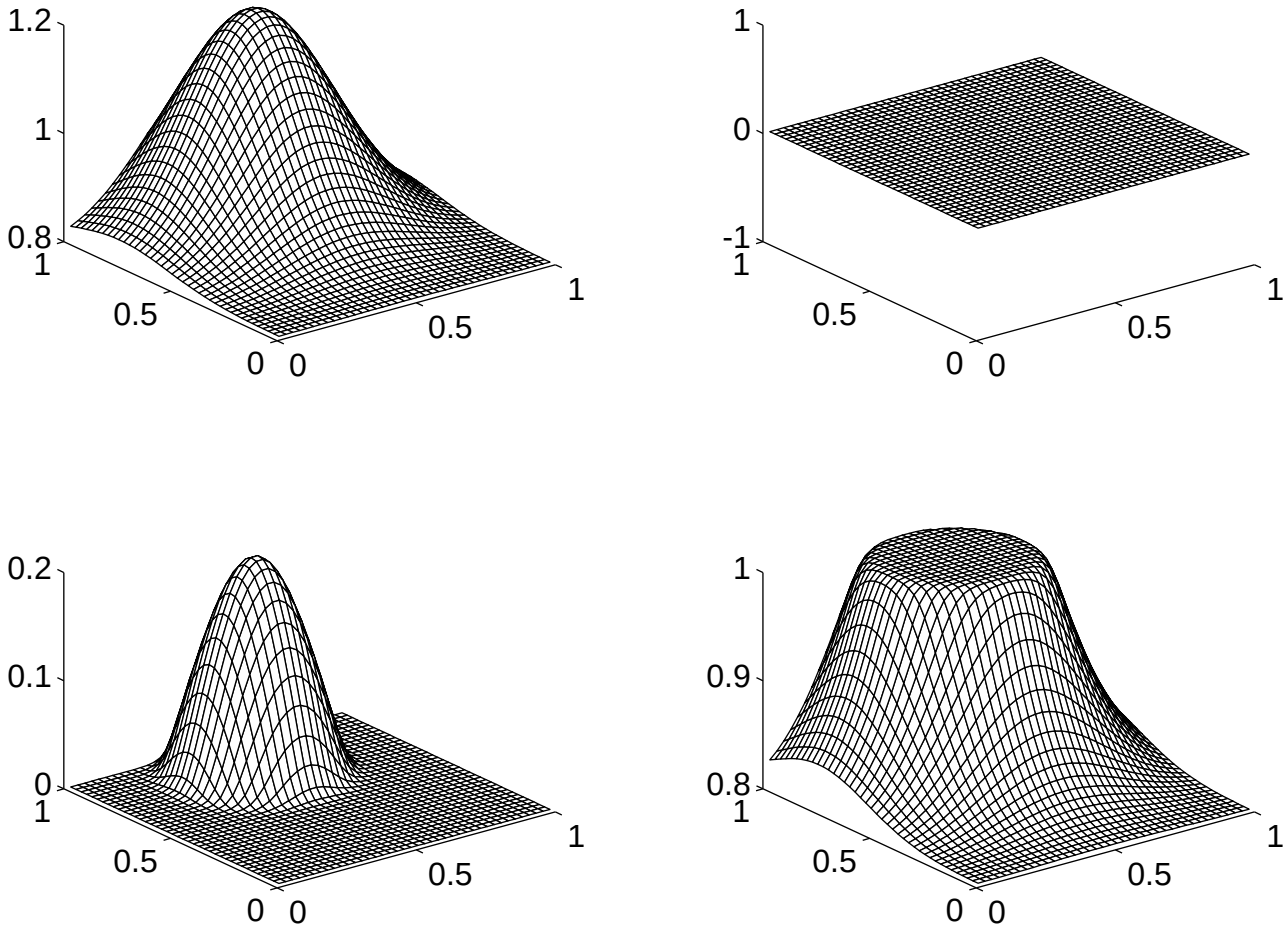

Figure 1. Solutions (6.3) at $t = 0$ (top) and $t = 1$ (bottom) after one rotation. Component $\mathbf{u_1}$ to the left and $\mathbf{u_2}$ to the right.

References

[1] R.M. Beam, R.F. Warming, *An implicit finite-difference algorithm for hyperbolic systems in conservation-law form.* J. Comp. Phys. 22, pp. 87-110 (1976).

[2] P. Brenner, M. Crouzeix, V. Thomée, *Single step methods for inhomogeneous linear differential equations.* RAIRO Numer. Anal. 16, pp. 5-26 (1982).

[3] R. Čiegis, K. Kiškis, *On the stability of LOD difference methods with respect to boundary conditions.* Lithuanian Academy of Sciences, Informatica 5, pp. 297-323 (1994).

[4] E. Hairer, S.P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I – Nonstiff Problems.* Springer Verlag, Berlin, 1987.

[5] P.J. van der Houwen, B.P. Sommeijer, *Splitting methods for three-dimensional transport models with interaction terms.* CWI Report NM-R9516, 1995.

[6] P.J. van der Houwen, J.G. Verwer, *One-step splitting methods for semi-discrete parabolic equations.* Computing 22, pp. 291-309 (1979).

[7] W. Hundsdorfer, *Unconditional convergence of some Crank-Nicolson methods for initial-boundary value problems.* Math. Comp. 58, pp. 35-53 (1992).

[8] W. Hundsdorfer, *A note on stability of the Douglas splitting method.* CWI Report, 1996.

[9] W. Hundsdorfer, J.G. Verwer, *Stability and convergence of the Peaceman-Rachford ADI method for initial-boundary value problems.* Math. Comp. 53, pp. 81-101 (1989).

[10] J.F.B.M Kraaijevanger, *B-convergence of the implicit midpoint rule and the trapezoidal rule.* BIT 25, pp. 652-666 (1985).

[11] R.J. LeVeque, *Intermediate boundary conditions for LOD, ADI and approximate factorization methods.* ICASE Report 85-21, Langley Research Center, 1985.

[12] Ch. Lubich, A. Ostermann, *Interior estimates for time discretization of parabolic equations.* Appl. Num. Math. 18, pp. 241-251 (1995).

[13] G.I. Marchuk, *Splitting and alternating direction methods.* Handbook of Numerical Analysis 1 (P.G. Ciarlet. J.L. Lions, eds.), North-Holland, Amsterdam, pp. 197-462, 1990.

[14] A.R. Mitchell, D.F. Griffiths, *The Finite Difference Method in Partial Differential Equations.* John Wiley & Sons, Chichester, 1980.

[15] J.G. Verwer, J.M. Sanz-Serna, *Convergence of method of lines approximations to partial differential equations.* Computing 33, pp. 297-313 (1984).

[16] N.N. Yanenko, *The Method of Fractional Steps.* Springer Verlag, Berlin, 1971.