A Fractional Step θ-method for Convection-Diffusion Problems

J.C. Chrispell * V.J. Ervin * E.W. Jenkins *

Abstract

In this article, we analyze the fractional-step θ method for the time-dependent convection-diffusion equation. In our implementation, we completely separate the convection operator from the diffusion operator, and stabilize the convective solve using a streamline upwinded Petrov-Galerkin (SUPG) method. We establish a priori error estimates and show that the optimal value of θ yield a scheme that is second order in time. Numerical computations are presented which demonstrate the method and support the theoretical results.

Key words. θ-method; splitting method; convection-diffusion

AMS Mathematics subject classifications. 65N30

Dedicated to Professor Bill Ames on the occasion of his 80th birthday.

1 Introduction

Modeling equations of mixed type often appear in physical applications. This paper is motivated by the work in [20], [21],[22] on the numerical approximation of viscoelastic fluid flow. The modeling equations (assuming *slow* flow) represent a "Stokes system" for the Conservation of Mass and Momentum equations, coupled with a non-linear hyperbolic equation describing the constitutive equation for the stress. The numerical approximation requires the determination of the fluid's velocity, pressure and stress (a symmetric tensor). For an accurate approximation a direct approximation technique requires the solution of a very large non-linear system of equations at each time step. The fractional step θ-method [22] decouples the approximation of velocity and pressure from the approximation of the stress, thereby reducing the size of the algebraic systems which have to be solved at each sub-step. An added benefit of the θ-method [22] is that the algebraic systems to be solved at each sub-step are linear.

In this paper we analyze the θ-method for the scalar convection-diffusion problem. This problem is chosen because the approximation scheme studied is similar to that in [22]. The middle sub-step in both applications is a pure convection (transport) problem, and the first and third sub-steps are parabolic problems.

*Department of Mathematical Sciences, Clemson University, Clemson, SC, 29634-0975, USA. email: `jchrisp@clemson.edu` `vjervin@clemson.edu` `lea@clemson.edu`. Partially supported by the NSF under grant no. DMS-0410792.

The fractional step θ-method was introduced, and its temporal approximation accuracy studied for a symmetric, positive definite spatial operator, by Glowinski and Pirreneau in [9]. The method is widely used for the accurate approximation of the Navier-Stokes equations (NSE) [23], [12]. In [16], Kloucek and Rys showed, assuming a unique solution existed, that the θ-method approximation converged to the solution of the NSE as the spatial and mesh parameters went to zero (h, $\Delta t \to 0_+$). The temporal discretization error for the θ-method for the NSE was studied by Müller-Urbaniak in [18] and shown to be second order.

The implementation of the fractional step θ-method in [22] for viscoelasticity differs significantly from that for the NSE. For the NSE at each sub-step the discretization contains the *stabilizing* operator $-\Delta \mathbf{u}$. For the viscoelasticity problem, and the convection-diffusion problem, analysed in this paper, the middle-substep is a pure convection (transport) problem.

Operator splitting methods for convection-diffusion problems can be divided into two approaches: (i) additive decomposition methods, and (ii) product decomposition methods. Additive decomposition methods rewrite the spatial operator as a sum of several operators. At each sub-step in the approximation algorithm the spatial operator is replaced by its additive decomposition, with some of the operators evaluated at the current time (i.e. treated implicitly) and the others at past times (i.e. treated explicitly). Examples of this approach are the Alternating Direction Implicit (ADI) methods [19],[14],[6],[17] and the IMplicit EXplicit (IMEX) schemes [1],[11]. With product decomposition methods, to advance the approximation from time t_{n-1} to t_n, firstly a pure convective operator is applied to obtain an initial estimate at t_n. This estimate is then taken as the initial data at t_{n-1} and a pure diffusion operator used to determine the approximation at t_n. Examples of this approach include the work of Dawson and Wheeler [5], [4], Khan and Liu [15], and Evje and Karlsen [8]. (See Section 4 in [7] for a survey of these methods.)

The fractional step θ-method we study is an additive decomposition method, with the desirable features of a product decomposition method. In the first and third sub-steps of the three sub-step algorithm a pure diffusion problem is approximated. In the second sub-step a pure convection problem is approximated.

This paper is organized as follows. In the next section we specify the problem we are studying and give the mathematical notation which we use. In Sections 3 and 4 we describe the fractional step θ-method for the convection-diffusion equation, show computability of the algorithm, and give the a priori error estimates for the method. A discussion on the optimal choice of the θ parameter is given in Section 5. Several numerical examples demonstrating the method are presented in Section 6.

2 Mathematical Problem and Notation

In this section we introduce the problem studied in this paper and the mathematical notation used. We also recall Gronwall's inequality which is used in the error analysis.

Below we study the numerical approximation of the following linear convection-diffusion equation using the fractional step θ-method.

$$\begin{aligned}
\frac{\partial u}{\partial t} - \triangle u + \mathbf{b}\cdot\nabla u + c\,u &= f \quad \text{in} \quad \Omega\times(0,T] && (2.1)\\
u(x,t) &= 0, \quad x\in\partial\Omega\times(0,T] && (2.2)\\
u(x,0) &= u_0(x), \quad x\in\Omega, && (2.3)
\end{aligned}$$

where $\mathbf{b} = [b_1(x,t), b_2(x,t)]^T$ is an incompressible velocity field (i.e $\nabla\cdot\mathbf{b} = 0$), $c(x,t) \geq c_0$ is an absorption coefficient, and $f(x,t)$ is a given body force.

The $L^2(\Omega)$ norm and inner product are denoted by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively. We use H^k to represent the Sobolev space W_2^k, and $\|\cdot\|_k$ denotes the norm in H^k. We let X denote the space $H_0^1(\Omega)$. When $v(\mathbf{x},t)$ is defined on the entire time interval $(0,T)$, we define

$$\|v\|_{\infty,k} := \sup_{0<t<T}\|v(\cdot,t)\|_k\ , \quad \|v\|_{0,k} := \left(\int_0^T\|v(\cdot,t)\|_k^2\,dt\right)^{1/2}\ , \quad \|v\|(t) := \|v(\cdot,t)\|\ .$$

We assume that $\Omega\subset\mathbb{R}^2$ is a polygonal domain and let T_h denote a regular triangulation of Ω. Thus, the computational domain is given by

$$\Omega = \cup K;\quad K\in T_h.$$

We assume that there exist constants c_1, c_2 such that

$$c_1 h \leq h_K \leq c_2\rho_K\ ,$$

where h_K is the diameter of triangle K, ρ_K is the diameter of the greatest ball (sphere) included in K, and $h = \max_{K\in T_h} h_K$. Let $P_k(A)$ denote the space of polynomials on A of degree no greater than k. Then we define the finite element space X_h as:

$$X_h := \left\{v\in X\cap C(\bar{\Omega}) : v|_K\in P_k(K),\ \forall K\in T_h\right\}\ .$$

Let $\mathcal{U}$ be the L^2 projection of u onto X_h, and use $u^{(n)} := u(\cdot, n\Delta t)$. Used in the error analysis are Λ^n and E^n defined by

$$\Lambda^n := u^n - \mathcal{U}^n\ , \qquad E^n := \mathcal{U}^n - u_h^n\ .$$

For $0\leq\theta\leq\frac{1}{2}$, we define the temporal operator $d_\theta u^{(n)}$ as

$$d_\theta u^{(n)} := \frac{u^{(n)} - u^{(n-\theta)}}{\theta\Delta t}.$$

The following discrete norms are used in the analysis.

$$|||v|||_{\infty,k} := \max_{1\leq n\leq N}\left\|v^{(n)}\right\|_k\ , \qquad |||v|||_{0,k} := \left(\sum_{n=1}^N\Delta t\left\|v^{(n)}\right\|_k^2\right)^{\frac{1}{2}}\ .$$

The discrete Gronwall inequality is used to establish a priori error estimates.

Lemma 2.1 ([10]) *Let $\Delta t, H,$ and a_n, b_n, c_n, γ_n (for integers $n \geq 0$) be nonnegative numbers such that*

$$a_l + \Delta t \sum_{n=0}^{l} b_n \leq \Delta t \sum_{n=0}^{l} \gamma_n a_n + \Delta t \sum_{n=0}^{l} c_n + H \quad \text{for } l \geq 0.$$

Suppose that $\Delta t \gamma_n < 1 \,\forall\, n$, and set $\sigma_n = (1 - \Delta t \gamma_n)^{-1}$. Then

$$a_l + \Delta t \sum_{n=0}^{l} b_n \leq \exp\left(\Delta t \sum_{n=0}^{l} \sigma_n \gamma_n\right) \left\{\Delta t \sum_{n=0}^{l} c_n + H\right\} \quad \text{for } l \geq 0. \tag{2.4}$$

3 The θ-method

The governing equation (2.1) can be represented abstractly as

$$\frac{\partial u}{\partial t} + F(u, x, t) = 0 \quad \text{in} \quad \Omega \times (0, T] \tag{3.1}$$

where

$$F(u, x, t) = -\triangle u + \mathbf{b} \cdot \nabla u + cu - f.$$

We split the operator $F(u, x, t)$ as

$$F(u, x, t) = F_1(u, x, t) + F_2(u, x, t) \tag{3.2}$$

where

$$F_1(u, x, t) \quad = \quad -\triangle u + \frac{c}{2} u - f \tag{3.3}$$

$$F_2(u, x, t) \quad = \quad \mathbf{b} \cdot \nabla u + \frac{c}{2} u. \tag{3.4}$$

Let $F^{(n)} := F\left(u^{(n)}, x, n\Delta t\right)$. We now describe a θ-method for the linear convection-diffusion problem.

Step 1: Given $u^{(n)}$, compute an approximation to $u^{(n+\theta)}$ by

$$d_\theta u^{(n+\theta)} + F_1^{(n+\theta)} = -F_2^{(n)} \tag{3.5}$$

Step 2: Given $u^{(n+\theta)}$, compute an approximation to $u^{(n+1-\theta)}$ by

$$d_{(1-2\theta)} u^{(n+1-\theta)} + F_2^{(n+1-\theta)} = -F_1^{(n+\theta)} \tag{3.6}$$

Step 3: Given $u^{(n+1-\theta)}$, compute an approximation to $u^{(n+1)}$ by

$$d_\theta u^{(n+1)} + F_1^{(n+1)} = -F_2^{(n+1-\theta)}. \tag{3.7}$$

Our corresponding discrete variation formulation to (3.5)–(3.7) is: *Determine $u_h^{(n+\theta)} \in X_h$, $u_h^{(n+1-\theta)} \in X_h$, and $u_h^{(n+1)} \in X_h$ satisfying*

$$\left(d_\theta u_h^{(n+\theta)} + \frac{c}{2} u_h^{(n+\theta)}, v\right) + \left(\nabla u_h^{(n+\theta)}, \nabla v\right) = \left(f^{(n+\theta)} - \mathbf{b} \cdot \nabla u_h^{(n)} - \frac{c}{2} u_h^{(n)}, v\right), \ \forall v \in X_h, \tag{3.8}$$

$$\left(d_{(1-2\theta)}u_h^{(n+1-\theta)}, v\right) + \left(\mathbf{b}\cdot\nabla u_h^{(n+1-\theta)} + \frac{c}{2}u_h^{(n+1-\theta)}, v_b\right) = \left(f^{(n+\theta)} - \frac{c}{2}u_h^{(n+\theta)}, v_b\right) - \left(\nabla u_h^{(n+\theta)}, \nabla v\right) + \left(\triangle u_h^{(n+\theta)}, \delta\mathbf{b}\cdot\nabla v\right), \ \forall v \in X_h, \quad (3.9)$$

$$\left(d_\theta u_h^{(n+1)} + \frac{c}{2}u_h^{(n+1)}, v\right) + \left(\nabla u_h^{(n+1)}, \nabla v\right) = \left(f^{(n+1)} - \mathbf{b}\cdot\nabla u_h^{(n+1-\theta)} - \frac{c}{2}u_h^{(n+1-\theta)}, v\right), \ \forall v \in X_h \quad (3.10)$$

Note: (i) To stabilize the convection (transport) equation (3.6), a Streamline Upwind Petrov Galerkin (SUPG) method is used. The term v_b is defined as $v_b \ := \ v \,+\, \delta\mathbf{b}\cdot\nabla v$.

(ii) The term $(\triangle u_h, \delta\mathbf{b}\cdot\nabla v)$ is defined *elementwise* as (see Johnson [13]):

$$(\triangle u_h, \delta\mathbf{b}\cdot\nabla v) \ := \ \sum_{K\in\mathcal{T}_h}\int_K \triangle u_h\,(\delta\mathbf{b}\cdot\nabla v)\;dA.$$

(iii) The solution $u(x,t)$ of (2.1),(2.2), satisfies the continuous variational formulation

$$(u_t, v) \,+\, (\nabla u, \nabla v) \,+\, (\mathbf{b}\cdot\nabla u, v) \,+\, (cu, v) \ = \ (f, v), \ \forall v \in X\,. \quad (3.11)$$

Remark: As mentioned previously, the θ-method described here differs from the approach used in [23],[12] for the numerical approximation of time-dependent Navier-Stokes equations in that in Step 2 of the above equation we are solving a pure transport problem. The investigation of this formulation is motivated by the application of the θ-method to time-dependent viscoelastic fluid flow problems, where such an approach leads to a decoupling of update equations for the stress and the velocity-pressure.

4 Analysis of the θ-method

The first step in the analysis of the method is to show that the scheme (3.8)–(3.10) is computable. That is, we need to show that the associated coefficient matrices on the left hand side of (3.8),(3.9), and (3.10) are invertible.

Lemma 1 *There exists a unique solution $u_h^{(n+\theta)} \in X_h$ satisfying (3.8).*

Proof: Equation (3.8) can be equivalently written as

$$\mathcal{A}(u_h^{(n+\theta)}, v_h) \ = \ \left(f^{(n+\theta)} + \frac{1}{\theta\Delta t}u_h^{(n)} - \mathbf{b}\cdot\nabla u_h^{(n)} - \frac{c}{2}u_h^{(n)}\,,\, v_h\right), \ \forall v_h \in X_h\,, \quad (4.12)$$

where

$$\mathcal{A}(w, z) \ = \ \frac{1}{\theta\Delta t}(w, z) \,+\, (\nabla w, \nabla z) \,+\, (\frac{c}{2}w, z)\,.$$

Note that (4.12) represents a square linear system of equations $A\mathbf{c} \ = \ \mathbf{f}$.

The fact that

$$\mathcal{A}(w, w) \ = \ \frac{1}{\theta\Delta t}(w, w) \,+\, (\nabla w, \nabla w) \,+\, (\frac{c}{2}w, w) \ > \ 0$$

guarantees that $ker(\mathcal{A}) = \{\mathbf{0}\}$. Hence it follows that (3.8) has a unique solution.

$\blacksquare$

The unique solvability of (3.10) follows exactly as for (3.8). For (3.9) the same approach, together with the divergence free assumption for $\mathbf{b}$ (i.e. $\nabla \cdot \mathbf{b} = 0$), establishes the unique solvability.

A priori error estimates

Having established the computability of the algorithm given in (3.8)-(3.10) we next address the question of the accuracy of the resulting approximation. This result is given in Theorem 1, and a discussion of its proof presented below. A detailed proof is given in [3].

Theorem 1 *For a sufficiently smooth solution u, with $\Delta t \leq Ch^2$ and $\delta \leq Ch$, the fractional step θ-scheme approximation, u_h given by (3.8)-(3.10), converges to u on the interval $(0,T]$ as $\Delta t, h \to 0$, and satisfies the error estimates:*

$$|||u - u_h|||_{0,1} \leq G(\Delta t, h, \delta) + Ch^k\,|||u|||_{\infty,k+1} \quad \text{and} \quad |||u - u_h|||_{\infty,0} \leq G(\Delta t, h, \delta) + Ch^{k+1}\,|||u|||_{\infty,k+1} \tag{4.13}$$

where

$$\begin{aligned} G(\Delta t, h, \delta) \;=\; & C(\Delta t)^2 \left(\|u_{ttt}\|_{0,0} + \|u_{tt}\|_{0,1} + \|u_{tt}\|_{0,0} + \|f_{tt}\|_{0,0} \right) \\ & + C\Delta t\, \delta \left(\|u_t\|_{0,2} + \|u_t\|_{0,1} + \|u_t\|_{0,0} + \|f_t\|_{0,0} \right) \\ & + Ch^{k+1}\,\|u_t\|_{0,k+1} + Ch^k\,|||u|||_{0,k+1} + C\delta\,|||u_t|||_{0,0} \end{aligned}$$

$\blacksquare$

Outline of the proof: To outline the proof of Theorem 1 it is instructive to review the procedure for obtaining an a priori estimate for an approximation scheme with a unit stride, i.e. only involving terms $u_h^{(0)}$, $u_h^{(1)}$, ..., $u_h^{(n)}$, $u_h^{(n+1)}$.

Step 1. Subtract the continuous and discrete variational equations and, after adding, subtracting terms and rearranging, obtain an expression of the form:

$$\left((u^{(n+1)} - u_h^{(n+1)}) - (u^{(n)} - u_h^{(n)})\,,\, v_h \right) + \frac{1}{2}\Delta t\, \mathcal{B}_{pos}((u^{(n+1)} - u_h^{(n+1)}), v_h) \;=\; \frac{1}{2}\Delta t\, \mathcal{B}_{rem}(\Delta t, f, u, u_h^{(n)}, v_h)\,,$$

where $\mathcal{B}_{pos}$ denotes the positive part of the operator.

Step 2. Use $u^{(n)} - u_h^{(n)} = \Lambda^{(n)} + E^{(n)}$, and choose $v_h = E^{(n+1)}$, to obtain an expression of the form

$$\left\| E^{(n+1)} \right\|^2 - \left\| E^{(n)} \right\|^2 + \frac{1}{2}\Delta t\, \mathcal{B}_{pos}(E^{(n+1)}, E^{(n+1)}) \;\leq\; \frac{1}{2}\Delta t\, \tilde{\mathcal{B}}_{rem}(\Delta t, f, u, \Lambda^{(n)}, \Lambda^{(n+1)}, E^{(n)}, E^{(n+1)})\,. \tag{4.14}$$

Equation (4.14) is then summed from $n = 0$ to $n = l - 1$ to obtain (assuming the $E^{(0)} = 0$)

$$\left\| E^{(l)} \right\|^2 + \Delta t \sum_{n=1}^{l} \mathcal{B}_{pos}(E^{(n)}, E^{(n)}) \;\leq\; \frac{1}{2}\Delta t\, \mathcal{R}(\Delta t, f, u, \Lambda^{(n)}, \Lambda^{(n+1)}, E^{(n)}, E^{(n+1)})\,. \tag{4.15}$$

Step 3. Apply suitable inequalities/estimates to the $\mathcal{B}_{pos}$ and $\mathcal{R}$ terms in (4.15).

Step 4. Apply Gronwell's lemma 2.1, with $a_l = \left\|E^{(l)}\right\|^2$ to obtain an estimate for $\left\|E^{(l)}\right\|$.

Step 5. Use the triangle inequality, $\|u^{(l)} - u_h^{(l)}\| \leq \|\Lambda^{(l)}\| + \|E^{(l)}\|$, and approximation properties to obtain the a priori estimate.

The term $\|\Lambda^{(l)}\|$ is estimated using interpolation properties.

Note that a key step in the analysis outlined in Steps 1–5 is the construction of the expression $\left\|E^{(n+1)}\right\|^2 - \left\|E^{(n)}\right\|^2$ which *telescopes* under summation to $\left\|E^{(l)}\right\|^2$.

With the θ-method there is **not** a uniform stride. Approximations $u_h^{(n+1)}$, $u_h^{(n+1-\theta)}$, and $u_h^{(n+\theta)}$ are computed. In order to generate appropriate telescoping expressions, linear combinations of equations (3.8), (3.9), and (3.10) need to be formed.

Step 1θ. Form the following linear combinations of equations (3.8), (3.9), and (3.10) to obtain equations involving $u_h^{(n+1)} - u_h^{(n)}$, $u_h^{(n+1-\theta)} - u_h^{(n-\theta)}$, and $u_h^{(n+\theta)} - u_h^{(n-1+\theta)}$, respectively.

$$\theta\,\Delta t\,(3.10) \;+\; (1-2\theta)\,\Delta t\,(3.9) \;+\; \theta\,\Delta t\,(3.8) \tag{4.16}$$
$$(1-2\theta)\theta\,\Delta t\,(3.9) \;+\; \theta\,\Delta t\,(3.8) \;+\; \theta\,\Delta t\,((3.10) \text{ with } n \to n-1) \tag{4.17}$$
$$\theta\,\Delta t\,(3.8) \;+\; \theta\,\Delta t\,((3.10) \text{ with } n \to n-1) \;+\; \theta\,\Delta t\,((3.9) \text{ with } n \to n-1)\,. \tag{4.18}$$

Subtract equations (4.16), (4.17), and (4.18), from (3.11), and after adding, subtracting terms and rearranging, to obtain equations

$$\begin{aligned}\Big((u^{(n+1)} - u_h^{(n+1)}) - (u^{(n)} - u_h^{(n)})\,,\, v_h\Big) \;+\; &\frac{1}{2}\Delta t\,\mathcal{G}_{pos}((u^{(n+1)} - u_h^{(n+1)}), v_h) \;=\\ &\frac{1}{2}\Delta t\,\mathcal{G}_{rem}(\Delta t, f, u, u_h^{(n+1-\theta)}, u_h^{(n+\theta)}, u_h^{(n)}, v_h)\,.\end{aligned}$$

$$\begin{aligned}\Big((u^{(n+1-\theta)} - u_h^{(n+1-\theta)}) - (u^{(n-\theta)} - u_h^{(n-\theta)})\,,\, v_h\Big) \;+\; &\frac{1}{2}\Delta t\,\mathcal{H}_{pos}((u^{(n+1-\theta)} - u_h^{(n+1-\theta)}), v_h) \;=\\ &\frac{1}{2}\Delta t\,\mathcal{H}_{rem}(\Delta t, f, u, u_h^{(n+\theta)}, u_h^{(n)}, u_h^{(n-\theta)}, v_h)\,.\end{aligned}$$

$$\begin{aligned}\Big((u^{(n+\theta)} - u_h^{(n+\theta)}) - (u^{(n-1+\theta)} - u_h^{(n-1+\theta)})\,,\, v_h\Big) \;+\; &\frac{1}{2}\Delta t\,\mathcal{K}_{pos}((u^{(n+\theta)} - u_h^{(n+\theta)}), v_h) \;=\\ &\frac{1}{2}\Delta t\,\mathcal{K}_{rem}(\Delta t, f, u, u_h^{(n)}, u_h^{(n-\theta)}, u_h^{(n-1+\theta)}, v_h)\,.\end{aligned}$$

Step 2θ. This step is similar to **Step 2** described above and equations for $\left\|E^{(l)}\right\|^2$, $\left\|E^{(l-\theta)}\right\|^2$, and $\left\|E^{(l-1+\theta)}\right\|^2$ are obtained. These three equations are then added together to form a single equation.

Step 3θ. Suitable inequalities/estimates are then applied to the terms in the equation.

Step 4θ. Gronwell's lemma is applied with $a_l = \left\|E^{(l)}\right\|^2 + \left\|E^{(l-\theta)}\right\|^2 + \left\|E^{(l-1+\theta)}\right\|^2$.

Step 5θ. The triangle inequality is applied to get the error estimate for $\left\|u^{(l)} - u_h^{(l)}\right\| + \left\|u^{(l-\theta)} - u_h^{(l-\theta)}\right\| + \left\|u^{(l-1+\theta)} - u_h^{(l-1+\theta)}\right\|$.

Below in Section 6 we present numerical results for a continuous, piecewise linear approximation to u. For this case (4.13) gives the following estimate.

Corollary 1 *For X_h the space of continuous, piecewise linear functions, $\Delta t \leq Ch^2$, $\delta \leq Ch$, and u sufficiently smooth, the approximation u_h satisfies the error estimate:*

$$|||u - u_h|||_{0,1} \;\leq\; C\left((\Delta t)^2 \,+\, \Delta t\,\delta \,+\, h \,+\, \delta\right) \quad \text{and } |||u - u_h|||_{\infty,0} \;\leq\; C\left((\Delta t)^2 \,+\, \Delta t\,\delta \,+\, h \,+\, \delta\right). \tag{4.19}$$

■

5 Optimal θ

In [9] Glowinski and Periaux studied the convergence and stability of the θ-method for

$$\frac{d\mathbf{u}}{dt} + A\mathbf{u} \;=\; \mathbf{0}\,,$$

where A was assumed to be a constant $p \times p$ symmetric, positive definite matrix and $\mathbf{u} \in \mathbb{R}^p$. The decomposition they considered (see (3.2)) was, for $\alpha \in (0, 1)$,

$$A\mathbf{u} \;=\; \alpha A\mathbf{u} + (1 - \alpha)A\mathbf{u},$$

i.e. $F_1(\mathbf{u}, t) \;=\; \alpha A\mathbf{u}$ and $F_2(\mathbf{u}, t) \;=\; (1 - \alpha)A\mathbf{u}$. Using an eigenvalue analysis, the authors were able to establish that for the choice $\theta = 1 - \sqrt{2}/2$ the fractional step θ-method was second order accurate in time, independent of the choice of α.

An eigenvalue analysis approach is not possible for the approximation method described in (3.8)–(3.10). In Step1θ of the analysis outlined above, the linear combinations given in (4.16),(4.17), and (4.18) give rise to expressions having the following forms.

- In $\mathcal{G}_{rem}$:

$$\theta u^{(n+1)} + (1-\theta)\, u^{(n+\theta)} - u^{\left(n+\frac{1}{2}\right)}\,,$$

$$(1-\theta)\, u^{(n+1-\theta)} + \theta u^{(n)} - u^{\left(n+\frac{1}{2}\right)}\,.$$

- In $\mathcal{H}_{rem}$:

$$\theta u^{(n)} + (1-\theta)\, u^{(n+\theta)} - u^{\left(n+\frac{1}{2}-\theta\right)}\,,$$

$$(1-2\theta)\, u^{(n+1-\theta)} + \theta u^{(n)} + \theta u^{(n-\theta)} - u^{\left(n+\frac{1}{2}-\theta\right)}\,.$$

- In $\mathcal{K}_{rem}$:

$$\theta u^{(n)} + (1-\theta)\, u^{(n-\theta)} - u^{\left(n+\theta-\frac{1}{2}\right)}\,,$$

$$(1-2\theta)\, u^{(n+\theta-1)} + \theta u^{(n)} + \theta u^{(n+\theta)} - u^{\left(n+\theta-\frac{1}{2}\right)}\,.$$

In order to obtain suitable estimates for these expressions, the terms are expanded in a Taylor series about $(n+1/2)\Delta t$, $(n+1/2-\theta)\Delta t$, and $(n+\theta-1/2)\Delta t$ for the $\mathcal{G}_{rem}$, $\mathcal{H}_{rem}$, and $\mathcal{K}_{rem}$ expressions, respectively. When this is done the first order terms in the expansions, i.e. the coefficients of Δt, all reduce to a constant multiple of

$$2\theta^2 \;-\; 4\theta \;+\; 1\,. \tag{5.1}$$

The roots of (5.1) are $\theta \;=\; 1 \pm \sqrt{2}/2$. Thus in order to have a second order temporal discretization error the only possible choice for θ satisfying $0 < \theta < 1/2$ is $\theta \;=\; 1 - \sqrt{2}/2$.

The optimal θ value was investigated numerically by calculating experimental convergence rates for the convection-diffusion problem given in (2.1)–(2.3) for $\mathbf{b} = [1,1]^T$, $c = 1.0$, $\Omega = (0,1) \times (0,1)$, X_h the space of continuous piecewise linear functions, and f and u_0 determinded by the true solution

$$u(x,y,t) \;=\; 10xy(1-x)(1-y)e^{x^{4.5}}(1-t^4)\,. \tag{5.2}$$

The meshes used in calculating the experimental convergence, illustrated in Figure 5.1, were obtained by dividing the spatial (h) and temporal (Δt) discretization parameters on each successive mesh by two. As the spatial discretization scheme is second order, we expect the experimental convergence rate to be determined by the temporal discretization. Figure 5.1 indicates that when $\theta = 1 - \sqrt{2}/2$ the method has second order convergence with respect to both h and Δt.

Figure 5.2 displays the error $|||u - u_h|||_{0,0}$ at $T = 1$ on a mesh with $\Delta t = 1/128$, and $h = \sqrt{2}/320$ for different values of θ. The smallest error corresponds with $\theta = 1 - \sqrt{2}/2$.

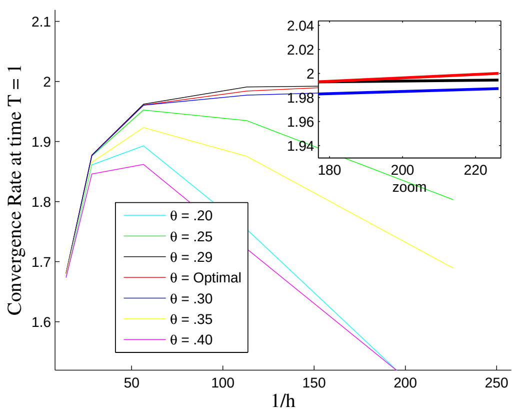

Figure 5.1: Experimental Convergence Rates.

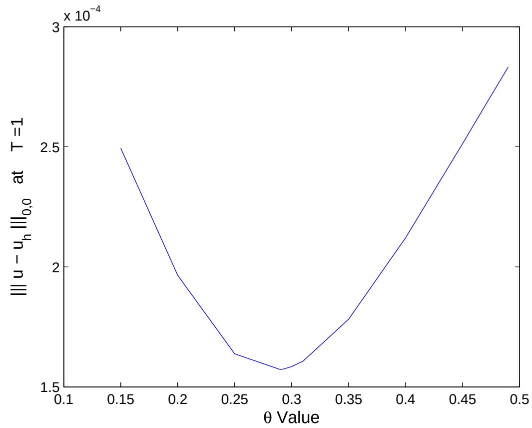

Figure 5.2: Error $|||u - u_h|||_{0,0}$ as a function of θ.

6 Numerical Computations

To demonstrate the fractional step θ-method (3.8)–(3.10) for convection diffusion problems, in this section we consider three examples. Example 1 is a simple convection-diffusion problem with a constant velocity field and a constant absorption coefficient. For Example 2 we consider a problem where the diffusion coefficient is several orders of magnitude less than the magnitude of the velocity field. The solution in Example 3 represents a steep moving front propagating through the domain. The value of θ used for the computations in this section was $\theta = 1 - \sqrt{2}/2$. For the three examples we compute a sequence of continuous, piecewise linear approximations u_h, by dividing the time step Δt and the spatial mesh parameter h by two. As the true solutions to the examples are known, we compute the experimental convergence rates (Cvge. Rate) for various choices of the parameter δ. As $\Delta t = Ch$, from Corollary 1, (4.19), the predicted convergence rates are $|||u - u_h|||_{0,1} \leq C(h+\delta)$, and $|||u - u_h|||_{\infty,0} \leq C(h+\delta)$. The numerical results obtained are consistent with these estimates.

In the proof of Theorem 1 the restriction $\Delta t \leq Ch^2$ is used. Computationally this is a very restrictive condition. For the numerical results obtained below we do not enforce this constraint. It is an open question if this condition is necessary for (4.13).

Example 1. For the model equations (2.1)–(2.3) we take $\mathbf{b} = [1, 1]^T$, $c = 1.0$, $\Omega = (0, 1) \times (0, 1)$, X_h the space of continuous piecewise linear functions, and f and u_0 determined by the true solution

$$u(x, y, t) \;=\; 10xy(1-x)(1-y)e^{x^{4.5}}(1-t^4)\,.$$

The solution is a slightly skewed bubble function which decays to zero at $t = 1$. The numerical results for this example are presented in Table 6.1.

	$\theta = 1 - \sqrt{2}/2$	Time $T = 1.0$				
$\delta \downarrow$	$(\Delta t, h) \rightarrow$	$(\frac{1}{10}, \frac{\sqrt{2}}{8})$	$(\frac{1}{20}, \frac{\sqrt{2}}{16})$	$(\frac{1}{40}, \frac{\sqrt{2}}{32})$	$(\frac{1}{80}, \frac{\sqrt{2}}{64})$	$(\frac{1}{160}, \frac{\sqrt{2}}{128})$
0	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{0,1}$	4.092e-1	2.184e-1	1.117e-1	5.628e-2	2.823e-2
	Cvge. Rate	-	0.9	1.0	1.0	1.0
	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{\infty,0}$	2.039e-2	5.358e-3	1.359e-3	3.411e-4	8.537e-5
	Cvge. Rate	-	1.9	2.0	2.0	2.0
h	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{0,1}$	5.407e-1	3.061e-1	1.576e-1	7.757e-2	3.772e-2
	Cvge. Rate	-	0.8	1.0	1.0	1.0
	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{\infty,0}$	7.055e-2	3.275e-2	1.524e-2	7.178e-3	3.443e-3
	Cvge. Rate	-	1.1	1.1	1.1	1.1
$h^{3/2}$	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{0,1}$	4.337e-1	2.259e-1	1.135e-1	5.668e-2	2.831e-2
	Cvge. Rate	-	0.9	1.0	1.0	1.0
	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{\infty,0}$	3.782e-2	1.176e-2	3.632e-3	1.138e-3	3.649e-4
	Cvge. Rate	-	1.7	1.7	1.7	1.6
h^2	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{0,1}$	4.124e-1	2.188e-1	1.117e-1	5.629e-2	2.823e-2
	Cvge. Rate	-	0.9	1.0	1.0	1.0
	$\lvert\lvert\lvert u - u_h\rvert\rvert\rvert_{\infty,0}$	2.613e-2	6.793e-3	1.709e-3	4.256e-4	1.058e-4
	Cvge. Rate	-	1.9	2.0	2.0	2.0

Table 6.1: Approximation errors and experimental convergence rates for Example 1.

Example 2. In this example, taken from [24], we consider the approximation of $u(x, y, t)$ satisfying

$$\frac{\partial u}{\partial t} \;-\; k\triangle u \;+\; \mathbf{b}\cdot\nabla u \;=\; f \quad \text{in} \quad \Omega \times (0, T]\,, \tag{6.1}$$

for $k = 0.0001$, $\mathbf{b} = [-4y, 4x]^T$, and $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$. For the solution we use

$$u(x, y, t) = \frac{2\sigma^2}{2\sigma^2 + 4kt} \exp\left(-\frac{(\bar{x} + 0.25)^2 + \bar{y}^2}{2\sigma^2 + 4kt}\right)\,, \tag{6.2}$$

with $\bar{x} = x\cos(4t) + y\sin(4t)$, $\bar{y} = -x\sin(4t) + y\cos(4t)$ and $\sigma = 0.0477$. The initial and boundary conditions used are given by $u_0(x, y) = u(x, y, 0)$, and $u(x, y, t)|_{\partial\Omega} = u(x, y, t) \approx 0$. The solution represents a Gaussian pulse being convected in a rotating velocity field. Table 6.2 lists the errors in the numerical approximation and the experimental convergence rates. The approximation is illustrated in Figures 6.1–6.4, for $h = \sqrt{2}/64$ and $\delta = h^2$.

	$\theta = 1 - \sqrt{2}/2$	Time $T = 0.3$				
$\delta \downarrow$	$(\Delta t, h) \rightarrow$	$(\frac{1}{10}, \frac{\sqrt{2}}{8})$	$(\frac{1}{20}, \frac{\sqrt{2}}{16})$	$(\frac{1}{40}, \frac{\sqrt{2}}{32})$	$(\frac{1}{80}, \frac{\sqrt{2}}{64})$	$(\frac{1}{160}, \frac{\sqrt{2}}{128})$
0	$\|\|\|u - u_h\|\|\|_{0,1}$	1.242e-0	7.999e-1	3.394e-1	1.543e-1	7.604e-2
	Cvge. Rate	-	0.6	1.2	1.1	1.0
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	8.114e-2	4.071e-2	1.127e-2	2.572e-3	6.338e-4
	Cvge. Rate	-	1.0	1.9	2.1	2.0
h	$\|\|\|u - u_h\|\|\|_{0,1}$	9.445e-1	7.978e-1	5.932e-1	4.079e-1	2.637e-1
	Cvge. Rate	-	0.2	0.4	0.5	0.6
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	6.609e-2	5.751e-2	4.353e-2	3.104e-2	2.057e-2
	Cvge. Rate	-	0.2	0.4	0.5	0.6
$h^{3/2}$	$\|\|\|u - u_h\|\|\|_{0,1}$	9.899e-1	7.375e-1	3.912e-1	1.797e-1	8.356e-2
	Cvge. Rate	-	0.4	0.9	1.1	1.1
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	6.619e-2	4.548e-2	2.135e-2	8.268e-3	3.003e-3
	Cvge. Rate	-	0.5	1.1	1.4	1.5
h^2	$\|\|\|u - u_h\|\|\|_{0,1}$	1.076e-0	7.519e-1	3.428e-1	1.553e-1	7.616e-2
	Cvge. Rate	-	0.5	1.1	1.1	1.0
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	7.102e-2	4.040e-2	1.281e-2	3.111e-3	7.702e-4
	Cvge. Rate	-	0.8	1.7	2.0	2.0

Table 6.2: Approximation errors and experimental convergence rates for Example 2.

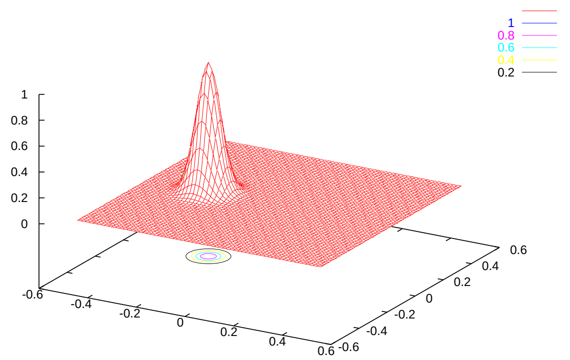

Figure 6.1: Example 2. Approximation u_h at $t = 0.0$

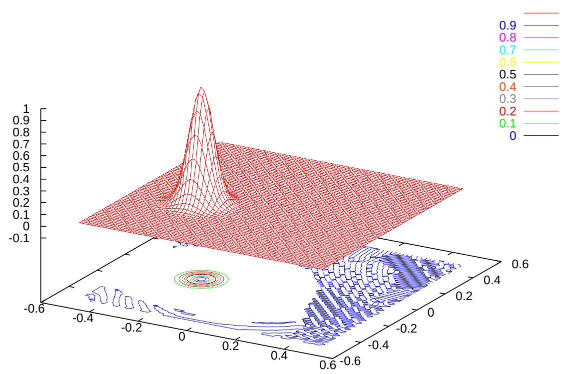

Figure 6.2: Example 2. Approximation u_h at $t = 0.1$

Example 3. In this example we consider the problem of approximating the solution to a moving front propagating through the domain, [2].

With $k = 0.01$, $f = 0$,

$$w(\eta, t) = \frac{0.1A + 0.5B + C}{A + B + C},$$

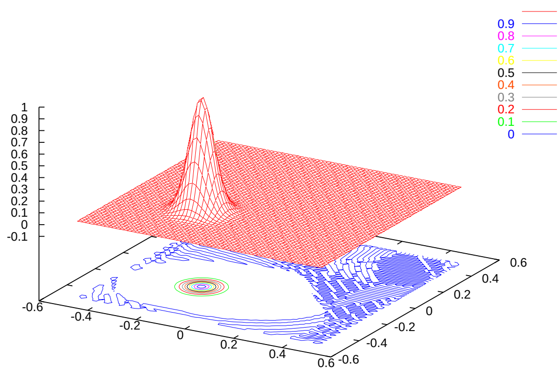

Figure 6.3: Example 2. Approximation u_h at $t = 0.2$

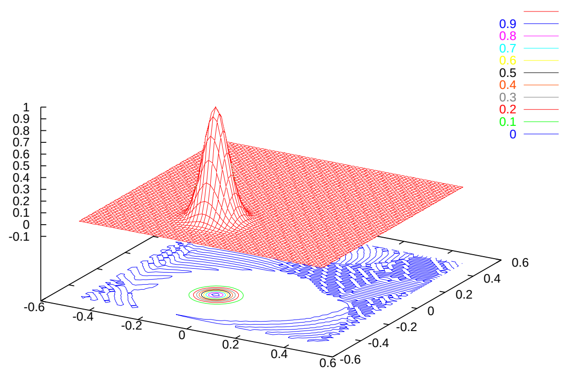

Figure 6.4: Example 2. Approximation u_h at $t = 0.3$

$$A(\eta, t) = \exp(-0.05(\eta - 0.5 + 4.95(t + 0.3))/k),\ B(\eta, t) = \exp(-0.25(\eta - 0.5 + 0.75(t + 0.3))/k)$$
$$C(\eta) = \exp(-0.5(\eta - 0.375)/k)$$

and $\mathbf{b} = [w(x,t), w(y,t)]^T$, $u(x, y, t)$ satisfying (6.1) is given by

$$u(x, y, t) \;=\; w(x, t)\, w(y, t)\,.$$

The boundary conditions and initial determined by the true solution, as in Example 2.

This example does not satisfy the assumptions for Theorem 1, as $\nabla \cdot \mathbf{b} \neq 0$. Nonetheless, the numerical results presented in Table 6.3 are consistent with those predicted in (4.13). Illustrated in Figures 6.5–6.8 is the numerical approximation computed using $h = \sqrt{2}/32$ and $\delta = h^{3/2}$.

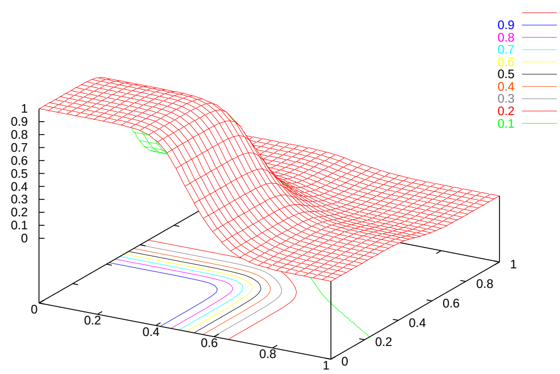

Figure 6.5: Example 3. Approximation u_h at $t = 0.0$

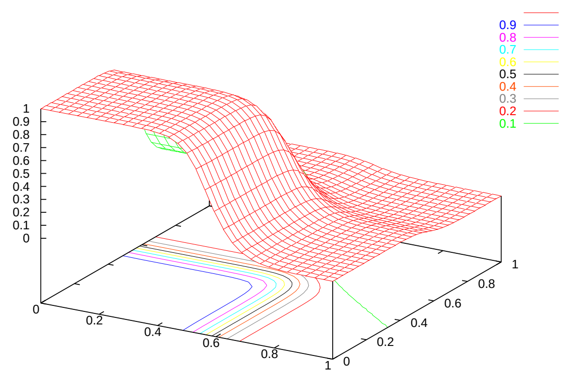

Figure 6.6: Example 3. Approximation u_h at $t = 0.1$

$\delta \downarrow$	$\theta = 1 - \sqrt{2}/2$ $(\Delta t, h) \rightarrow$	Time $T = 0.3$ $(\frac{1}{10}, \frac{\sqrt{2}}{8})$	$(\frac{1}{20}, \frac{\sqrt{2}}{16})$	$(\frac{1}{40}, \frac{\sqrt{2}}{32})$	$(\frac{1}{80}, \frac{\sqrt{2}}{64})$	$(\frac{1}{160}, \frac{\sqrt{2}}{128})$
0	$\|\|\|u - u_h\|\|\|_{0,1}$	5.193e-1	2.722e-1	1.301e-1	6.389e-2	3.163e-2
	Cvge. Rate	-	0.9	1.1	1.0	1.0
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	4.032e-2	1.663e-2	6.805e-3	3.214e-3	1.576e-3
	Cvge. Rate	-	1.3	1.3	1.1	1.0
h	$\|\|\|u - u_h\|\|\|_{0,1}$	4.775e-1	2.999e-1	1.684e-1	9.099e-2	4.761e-2
	Cvge. Rate	-	0.7	0.8	0.9	0.9
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	4.693e-2	2.819e-2	1.580e-2	8.642e-3	4.561e-3
	Cvge. Rate	-	0.7	0.8	0.9	0.9
$h^{3/2}$	$\|\|\|u - u_h\|\|\|_{0,1}$	4.659e-1	2.586e-1	1.267e-1	6.263e-2	3.113e-2
	Cvge. Rate	-	0.8	1.0	1.0	1.0
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	4.054e-2	1.730e-2	6.900e-3	3.114e-3	1.503e-3
	Cvge. Rate	-	1.2	1.3	1.1	1.1
h^2	$\|\|\|u - u_h\|\|\|_{0,1}$	4.867e-1	2.656e-1	1.289e-1	6.362e-2	3.156e-2
	Cvge. Rate	-	0.9	1.0	1.0	1.0
	$\|\|\|u - u_h\|\|\|_{\infty,0}$	3.975e-2	1.644e-2	6.704e-3	3.175e-3	1.565e-3
	Cvge. Rate	-	1.3	1.3	1.1	1.0

Table 6.3: Approximation errors and experimental convergence rates for Example 3.

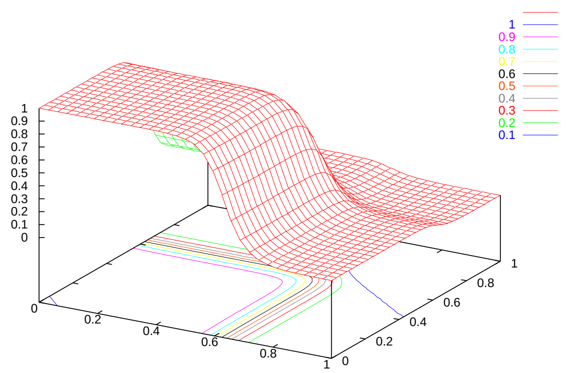

Figure 6.7: Example 3. Approximation u_h at $t = 0.2$

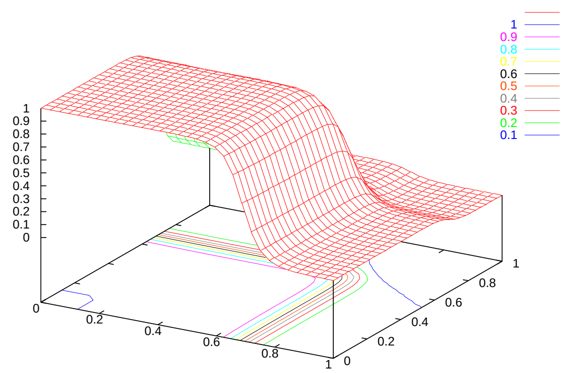

Figure 6.8: Example 3. Approximation u_h at $t = 0.3$

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