A novel Exponential Time Differencing (ETD) Crank-Nicolson method is developed which is stable, second order convergent, and highly efficient. We prove stability and convergence for semilinear parabolic problems with smooth data. In the nonsmooth data case we employ a positivity-preserving initial damping scheme to recover the full rate of convergence. Numerical experiments are presented for a wide variety of examples, including chemotaxis and exotic options with transaction cost.

Keywords: Exponential Time Differencing, transaction cost, exotic options, nonlinear Black-Scholes equation, chemotaxis

I. INTRODUCTION

Various types of Exponential Time Differencing Runge-Kutta schemes (ETDRK) for nonlinear parabolic equations have been proposed and investigated, though there is no complete theoretical analysis and the focus has not been on any specific efficient version like the one introduced in this article. This Exponential Time Differencing Crank-Nicolson (ETD-CN) scheme utilizes an exponential time differencing Runge-Kutta approach followed by a (1,1)–diagonal
Padé approximation of matrix exponential functions. This is an extension of several previous papers on Exponential Time Differencing schemes, in particular [4, 6, 9, 10, 19, 20, 22].

Once we define the nonlinear reaction-diffusion problem and develop the algorithm in Sections II. and III., we prove stability and convergence in Section IV. In Sections V. and VI. we demonstrate the highly efficient performance through solving various important nonlinear problems from the literature. Finally, Section VII. contains a short summary and conclusion.

II. THE REACTION-DIFFUSION SYSTEM

Consider the following nonlinear parabolic initial-boundary value problem:

\[ u_t + Au = F(t, u) \quad \text{in } \Omega, \quad t \in (0, T), \]

\[ u(\cdot, 0) = u_0 \quad \text{in } \Omega, \]

where \( \Omega \) is a bounded domain in \( \mathbb{R}^d \) with Lipschitz continuous boundary, \( A \) represents a uniformly elliptic operator, and \( F \) is a sufficiently smooth, nonlinear reaction term. One should have in mind the following type of differential operator:

\[
A := - \sum_{j,k=1}^{d} \frac{\partial}{\partial x_j} \left( a_{j,k}(x) \frac{\partial}{\partial x_k} \right) + \sum_{j=1}^{d} b_j(x) \frac{\partial}{\partial x_j} + b_0(x),
\]

where the coefficients \( a_{j,k} \) and \( b_j \) are \( C^\infty \) (or sufficiently smooth) functions on \( \bar{\Omega} \), \( a_{j,k} = a_{k,j} \), \( b_0 \geq 0 \), and for some \( c_0 > 0 \)

\[
\sum_{j,k=1}^{d} a_{j,k}(\cdot) \xi_j \xi_k \geq c_0 |\xi|^2, \quad \text{on } \bar{\Omega}, \quad \text{for all } \xi \in \mathbb{R}^d.
\]

However, we shall use \( A \) and \( F \) based on an abstract formulation for convenience of the development of the numerical scheme and its analysis. The initial value problem (2.1) is reset to be posed in a Banach space \( \mathcal{X} \), as follows. Consider now \( A \) to be a linear, self-adjoint, positive definite, closed operator with a compact inverse, defined on a dense domain \( D(A) \subset \mathcal{X} \). The operator \( A \) could represent any of \( \{A_h\}_{0 < h \leq h_0} \), obtained through spatial discretization, and \( \mathcal{X} \) could be \( \mathcal{X} = \mathcal{S}_h \), an appropriate finite dimensional subspace of \( L^2(\Omega) \), cf. [3, 23, 26, 32].

We assume the resolvent set \( \rho(A) \) satisfies, for some \( \alpha \in (0, \frac{\pi}{2}) \), \( \rho(A) \supset \Sigma_\alpha \), where \( \Sigma_\alpha := \{z \in \mathbb{C} : \alpha < \arg(z) \leq \pi, z \neq 0\} \). Also, assume there exists \( M \geq 1 \) such that

\[
\|(zI - A)^{-1}\| \leq M|z|^{-1}, \quad z \in \Sigma_\alpha.
\]
It follows that $-A$ is the infinitesimal generator of an analytic semigroup $\{e^{-tA}\}_{t \geq 0}$ which is the solution operator for (2.1), cf. [7, 23, 26], and $\|e^{-tA}\|_X \leq C$ for $t \geq 0$.

Using Cauchy’s Integral Formula we obtain the standard representation

$$E(t) := e^{-tA} = \frac{1}{2\pi i} \int_{\Gamma} e^{\tau z} (zI - A)^{-1} dz,$$  \hspace{1cm} (2.3)

where $\Gamma := \{ z \in \mathbb{C} : |\arg(z)| = \theta \}$, oriented so that $\text{Im}(z)$ decreases, for any $\theta \in (\alpha, \frac{\pi}{2})$.

Furthermore, we assume cf. [18, Remark 1.1, p. 324] that $D$ is a locally closed subset of $X$ and $F : [0, \infty) \times D \to X$ is continuous. Then, it follows that for $z \in D$ there are positive numbers $R, M,$ and $T$ such that

$$S_R \equiv \{ x \in D : \|x - z\| \leq R \} \text{ is closed},$$

$$\|F(t, x)\| \leq M - 1, \quad \text{if } (t, x) \in [0, T] \times S_R, \quad \text{and} \quad \|E(t)z + y - z\| \leq R/2, \quad \text{if } t \in [0, T] \text{ and } y \in X \text{ with } \|y\| \leq T(M - 1)e^{\omega T},$$  \hspace{1cm} (2.4)

where $\omega$ is the least number such that $\|E(t)\| \leq e^{\omega t} \forall t \geq 0$.

We also assume that $x \in S_R$ implies $E(t)x \in D$, $\forall t \in [0, T]$ and that

$$\lim \inf_{h \to 0^+} \frac{d(x + hF(t, x); D)}{h} = 0, \quad \forall (t, x) \in [0, T] \times D.$$  

By the Duhamel principle we know that each solution of (2.1) must be of the form

$$u(t) = E(t)u_0 + \int_0^t E(t - s) F(s, u(s)) \, ds.$$  \hspace{1cm} (2.5)

Under the assumptions made, we have (cf. [18, Theorem 2.1, p. 335] and [18, Remark 2.1, p. 337], respectively)

**Proposition 2.1.** If there is a number $L > 0$ such that $\|F(t, x) - F(t, y)\| \leq L\|x - y\|$ for all $(t, x), (t, y) \in [0, T] \times S_R$, then (2.5) has a unique solution $u$ on $[0, T]$ with values in $D$.

So assume

**Assumption 2.1.** Let $F : [0, T] \times X \to X$ and $U$ be an open subset of $[0, T] \times X$. For every $(t, x) \in U$ there exists a neighborhood $V \subset U$ and a real number $L_T$ such that

$$\|F(t_1, x_1) - F(t_2, x_2)\|_X \leq L_T \left( |t_1 - t_2| + \|x_1 - x_2\|_X \right)$$  \hspace{1cm} (2.6)

for all $(t_1, x_1) \in V$.

For the proof below it is sufficient that (2.6) holds in a strip along the exact solution.

Let $0 < k \leq k_0$, for some $k_0$, and $t_n = nk$, $0 \leq n \leq N$. Replacing $t$ by $t + k$, using basic properties of $E$ and by the change of variable $s - t = k\tau$, we arrive at the following recurrence
formula for the exact solution:

\[
    u(t_{n+1}) = e^{-kA}u(t_n) + k \int_0^1 e^{-kA(1-\tau)}F(t_n + \tau k, u(t_n + \tau k)) \, d\tau.
\]  

(2.7)

This is the basis for deriving ETD schemes.

III. THE TIME STEPPING SCHEME ETD-CN

There are several ways of approximating the integral representation of the exact solution (2.7). Cox and Matthews [4] developed time stepping schemes by using polynomial formulae which give a Runge-Kutta type higher order approximation. Du and Zhu [6] and Kassam and Trefethen [14], and Nie, Zhang, and Zhao [22] pointed out some implementation difficulties. These ETD schemes are studied in many articles, cf., [6, 9, 10, 12, 19, 20, 28].

Prior treatments of ETD methods do not discretize the matrix exponentials, or else employ contour integration techniques. In this work we focus on the development of a highly efficient scheme by employing Padé approximations for some crucial terms. The proofs given in previous articles omit the fully discrete case, thus leaving a gap in the convergence theory. In this section we derive a highly efficient, fully discrete second order version of the ETD schemes and in the next section we address the theory.

We will approximate \( e^{-kA} \) using the \((0,1)−\) and \((1,1)−\) Padé schemes, \( R_{0,1}(kA) \) and \( R_{1,1}(kA) \), respectively, as follows. Specifically, we define \( R_{0,1}(kA) := (I + kA)^{-1} \) and \( R_{1,1}(kA) := (2I - kA)(2I + kA)^{-1} \), which is commonly called the ‘Crank-Nicolson,’ or CN, scheme.

Denoting the semi-discrete approximation to \( u(t_n) \) by \( u_n \) (note that only the time-variable is discretized) and \( F(t_n, u_n) \) by \( F_n \), the simplest approximation to the integral is to impose that \( F \) is constant for \( t \in [t_n, t_{n+1}] \), i.e. \( F \approx F_n \). This yields (from (2.7))

\[
    u_{n+1} \approx e^{-kA}u_n + e^{-kA}k \int_0^1 e^{kA\tau} \, d\tau F_n
    = e^{-kA}u_n - A^{-1}(e^{-kA} - I) F_n.
\]  

(3.1)

This semi-discrete scheme cf. [4, 19, 20] is not useful until the matrix exponential is discretized. Noting that

\[
    -A^{-1}(e^{-kA} - I) \approx -A^{-1}((I + kA)^{-1} - I)
    = -A^{-1}(I - (I + kA))(I + kA)^{-1}
    = k(I + kA)^{-1}
    = kR_{0,1}(kA),
\]  

(3.2)
we arrive at the following fully discrete first order scheme, where $v$ now denotes the fully discrete solution. This is the same as a standard first order linearly implicit scheme, in particular, [4, 6, 9, 10], the interesting aspect now being that this ETD derivation leads to an extended family of similar type of ETD schemes.

**Derivation of ETD-CN.** To obtain a second order accurate RK-scheme, we employ (3.1) as intermediate prediction of $u(t_{n+1})$, letting

$$a_n := e^{-kA}u_n - A^{-1}(e^{-kA} - I)F(t_n, u_n).$$

We then approximate the integral in (2.7) by

$$F \approx F_n + (t - t_n)\frac{F(t_n + k, a_n) - F_n}{k} \quad t \in [t_n, t_{n+1}].$$

Using (2.7), a short calculation yields the following:

$$u_{n+1} = e^{-kA}u_n + ke^{-kA}\int_{0}^{1}e^{kA\tau} \left(F_n + k\tau\frac{F(t_n + k, a_n) - F_n}{k}\right) d\tau
= a_n + \frac{1}{k}A^{-2}(e^{-kA} - I + kA)(F(t_n + k, a_n) - F(t_n, u_n)).$$

**The Second Order ETD Semi-discrete Scheme.** Thus a second order exponential time differencing Runge-Kutta semi-discrete type scheme is given by

$$u_{n+1} = a_n + \frac{1}{k}A^{-2}(e^{-kA} - I + kA)(F(t_n + k, a_n) - F(t_n, u_n)) \quad (3.3)$$

where

$$a_n = e^{-kA}u_n - A^{-1}(e^{-kA} - I)F(t_n, u_n). \quad (3.4)$$

The computational challenge now is to efficiently compute terms like $-A^{-1}(e^{-kA} - I)$ and $\frac{1}{k}A^{-2}(e^{-kA} - I + kA)$. Kassam and Trefethen [14] and Du and Zhu [6] have developed a contour integration technique for this problem [6, 14], while Hochbruck and Osterman [9, 10] do not deal with the problem, leaving the computation of polynomial functions of matrix exponentials to standard software at the time of implementation. The approach we introduce in this work deals directly with the full discretization of the underlying matrix exponentials with an eye on efficiency. Tests show that the fully-discrete ETD-CN version performs with significantly less CPU time than using a standard routine for the exponential of $A$. 

**FINAL VERSION** March 14, 2011, 7:27am
Similar to (3.2), except now with $R_{1,1}(kA)$ instead of $R_{0,1}(kA)$ for $e^{-kA}$ to achieve higher spatial accuracy, we compute that

$$-A^{-1}(e^{-kA} - I) \approx -A^{-1}[(2I - kA)(2I + kA)^{-1} - I]$$

$$= 2k(2I + kA)^{-1}$$

$$= kR_{0,1}\left(\frac{1}{2}kA\right),$$

(3.5)

and

$$\frac{1}{k}A^{-2}(e^{-kA} - I + kA) \approx \frac{1}{k}A^{-2}[(2I - kA)(2I + kA)^{-1} - I + kA]$$

$$= k(2I + kA)^{-1}.$$  (3.6)

In the expression (3.4) for $a_n$ we now use $b_n$ in order to distinguish between the semi-discrete case (with $e^{-kA}$) and the fully discrete predictor stage where $e^{-kA}$ is replaced by an appropriate Padé approximation. Next, we substitute (3.5, 3.6) into (3.3, 3.4), which gives the ETD-CN scheme:

$$v_{n+1} = b_n + \frac{1}{2}kR_{0,1}\left(\frac{1}{2}kA\right)\left[F(t_n + k, b_n) - F(t_n, v_n)\right],$$

(3.7)

$$b_n = R_{1,1}(kA)v_n + kR_{0,1}\left(\frac{1}{2}kA\right)F(t_n, v_n).$$

(3.8)

IV. PROOF OF CONVERGENCE FOR THE ETD-CN SCHEME

Several schemes based on Runge-Kutta time stepping were developed, cf. [4, 6, 9, 10, 14]. A complete proof of convergence is not attained to-date, as the fully discrete scheme is ignored, i.e., the matrix exponentials are left in primitive form. The convergence proof is not complete until it applies to the fully discrete scheme. It has been established through many important examples [15, 17, 24, 25, 29, 30, 31, 32], that nonsmooth initial data or mismatched initial-boundary conditions constitute an important class of application problems that should be addressed.

We will derive error bounds for the nonlinear parabolic problem (2.1) with time-independent operator $A$. For the proof of convergence we will need a discrete Gronwall Lemma.
Lemma 4.1. Suppose \( \varphi, \Psi \) satisfy 
\[
\delta \varphi(t_j) - c_1 \varphi(t_{j-1}) \leq \Psi(t_j) \text{ where } \delta \varphi(t_j) = \frac{\varphi(t_j) - \varphi(t_{j-1})}{k}.
\]
Then there is a constant \( C \) such that for sufficiently small \( k_0 \)
\[
\varphi(t_n) \leq C \left( \varphi(t_0) + k \sum_{j=1}^{n} \Psi(t_j) \right), \quad t_n = nk, \quad k \in (0, k_0).
\]

The semi-discrete case is covered in the following established result:

Theorem 4.2. (Hochbruck and Osterman [9]) Let the initial value problem (2.1) satisfy the assumptions listed and let \( F \in C^2([0, T]; L^1) \). Then, for sufficiently small time step \( k \), there exists a unique numerical solution \( u_n \) \((0 \leq nk \leq T), n \geq 0 \) whose error, if approximated by (3.3,3.4), satisfies
\[
\parallel u_n - u(t_n) \parallel_X \leq C k^2 \left( \sup_{0 \leq \tau \leq t_n} \parallel F(\tau, u(\tau)) \parallel_X + \sup_{0 \leq \tau \leq t_n} \parallel F^{(2)}(\tau, u(\tau)) \parallel_X \right).
\]
The constant \( C \) depends on \( T \), but is independent of \( n, k \), and \( A \).

The Hochbruck and Osterman theorem leaves out the case where the matrix exponentials are discretized. We now need to examine how to extend their proof [9] for \((1,1)\)-Padé discretization of these matrix exponentials.

Let us now consider the difference between the semi-discrete scheme (3.3, 3.4) and the fully discrete version (3.7, 3.8).

The Lipschitz continuity (2.6) of \( F(t, u) \) implies
\[
\parallel F(t, u) \parallel_X - \parallel F(t, v) \parallel_X \leq \parallel F(t, u) - F(t, v) \parallel_X \leq L \parallel u - v \parallel_X,
\]
i.e. in particular
\[
\parallel F(t, u) \parallel_X \leq L \parallel u \parallel_X + \parallel F(t, 0) \parallel_X \leq L \parallel u \parallel_X + D \tag{4.1}
\]
for a constant \( D = \max_{t \in [0,T]} \{\parallel F(t, 0) \parallel_X \} \), which is independent of \( u \).

Before we state the convergence result we need some estimates. We utilize the symbol \( C \) to indicate various upper bounds which are only allowed to depend on \( T, A \) or \( F \). The following lemma shows stability:

Lemma 4.3. Let the initial value problem (2.1) satisfy the listed assumptions, then
\[
\parallel u_n \parallel_X \leq CD + C \parallel u_0 \parallel_X.
\]
Proof. We have

\[ a_n = e^{-kA}u_{n-1} - A^{-1}(e^{-kA} - I)F(t_{n-1}, u_{n-1}) \]

\[ = e^{-kA}u_0 + k^{-1}A^{-2}(e^{-kA} - I + kA) \]

\[ + \sum_{j=1}^{n-1} e^{-jKA}(F(t_{n-j}, a_{n-j}) - F(t_{n-j-1}, u_{n-j})) \]

\[ - A^{-1}(e^{-kA} - I) \sum_{j=1}^{n-1} e^{-jKA}F(t_{n-j-1}, u_{n-j-1}) \]

\[ - A^{-1}(e^{-kA} - I)F(t_{n-1}, u_{n-1}) \quad (4.2) \]

using (3.3) and (3.4), and thus

\[ \|a_n\|_X \leq C\|u_0\|_X + \frac{Ck}{n-1} \sum_{j=1}^{n-1} \|a_{n-j} - a_{n-j-1}\|_X + Ck \sum_{j=0}^{n-1} \|u_j\|_X + CD, \]

where the parameter \( D \) is defined at (4.1). This yields

\[ \|u_n\|_X \leq \|a_n\|_X + \frac{1}{k} \|A^{-2}(e^{-kA} - I + kA)\|_X \|F(t_n, a_{n-1}) - F(t_{n-1}, u_{n-1})\|_X \]

\[ \leq C\|u_0\|_X + Ck \sum_{j=1}^{n-1} \|a_{n-j} - a_{n-j-1}\|_X + Ck \sum_{j=0}^{n-1} \|u_j\|_X + CD \]

\[ + CkL(\|t_n - t_{n-1}\|_X + \|a_{n-1} - u_{n-1}\|_X) \]

\[ \leq C\|u_0\|_X + Ck \sum_{j=1}^{n-1} \|a_j - u_j\|_X + Ck \sum_{j=0}^{n-1} \|u_j\|_X + CD \]

using (2.6). Also,

\[ \|a_j - u_j\|_X \leq \|e^{-kA} - I\|_X \|u_j\|_X + \|A^{-1}(e^{-kA} - I)F(t_j, u_j)\|_X \]

\[ \leq C\|u_j\|_X + CDk \quad (4.3) \]

yields

\[ \|u_n\|_X \leq Ck \sum_{j=0}^{n-1} \|u_j\|_X + CD + C\|u_0\|_X. \]

Now we can apply Gronwall’s Lemma 4.1 with \( \varphi(t_n) = k\sum_{j=0}^{n-1} \|u_j\|_X \) and \( \Psi(t_n) = CD + C\|u_0\|_X \) to obtain \( \|a_n\|_X \leq CD + C\|u_0\|_X \).

We will also need a similar estimate for \( Au_n \), namely
Lemma 4.4. Let the initial value problem (2.1) satisfy the listed assumptions as well as $F(t, u(t)) \in D(A)$, then

$$
\|Au_n\|_{\mathcal{X}} \leq C \|Au_0\|_{\mathcal{X}} + C \|u_0\|_{\mathcal{X}} + CD + Ck \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{\mathcal{X}}.
$$

(4.4)

Proof. We have

$$
\|Au_n\|_{\mathcal{X}} \leq \|Au_{n-1}\|_{\mathcal{X}} + \frac{1}{k} \|A^{-1}(e^{-kA} - I + kA)\|_{\mathcal{X}} \|F(t_n, a_{n-1}) - F(t_{n-1}, u_{n-1})\|_{\mathcal{X}}
$$

$$
\leq C \|Au_0\|_{\mathcal{X}} + C \sum_{j=1}^{n-1} \|a_{n-j-1} - u_{n-j-1}\|_{\mathcal{X}} + Ck \sum_{j=0}^{n-1} \|AF(t_{n-j-1}, u_{n-j-1})\|_{\mathcal{X}}
$$

$$
+ CD + CL (|t_n - t_{n-1}| + \|a_{n-1} - u_{n-1}\|_{\mathcal{X}})
$$

$$
\leq C \|Au_0\|_{\mathcal{X}} + C \sum_{j=0}^{n-1} \|a_j - u_j\|_{\mathcal{X}} + Ck \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{\mathcal{X}} + CD.
$$

using (2.6) and (by (4.2))

$$
\|Aa_{n-1}\|_{\mathcal{X}} \leq C \|Au_0\|_{\mathcal{X}} + C \sum_{j=1}^{n-1} \|a_{n-j-1} - u_{n-j-1}\|_{\mathcal{X}}
$$

$$
+ Ck \sum_{j=0}^{n-1} \|AF(t_{n-j-1}, u_{n-j-1})\|_{\mathcal{X}} + CD.
$$

Here we use

$$
\|a_j - u_j\|_{\mathcal{X}} \leq \|A^{-1}(e^{-kA} - I)\|_{\mathcal{X}} \|Au_j\|_{\mathcal{X}} + \|A^{-1}(e^{-kA} - I)F(t_j, u_j)\|_{\mathcal{X}}
$$

$$
\leq Ck \|Au_j\|_{\mathcal{X}} + Ck \|u_j\|_{\mathcal{X}} + CDk
$$

(4.5)

instead of (4.3) to obtain

$$
\|Au_n\|_{\mathcal{X}} \leq C \|Au_0\|_{\mathcal{X}} + Ck \sum_{j=0}^{n-1} \|Au_j\|_{\mathcal{X}} + Ck \sum_{j=0}^{n-1} \|u_j\|_{\mathcal{X}}
$$

$$
+ Ck \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{\mathcal{X}} + CD
$$

$$
\leq C \|Au_0\|_{\mathcal{X}} + C \|u_0\|_{\mathcal{X}} + Ck \sum_{j=0}^{n-1} \|Au_j\|_{\mathcal{X}}
$$

$$
+ Ck \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{\mathcal{X}} + CD
$$

by Lemma 4.3.
Now we can apply Gronwall’s Lemma 4.1 with \( \varphi(t_n) = k \sum_{j=0}^n \|Au_j\|_X \) and \( \Psi(t_n) = C \|Au_0\|_X + C \|u_0\|_X + CK \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X + CD \) to obtain

\[
\|Au_n\|_X \leq C \|Au_0\|_X + C \|u_0\|_X + CD + CK \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X. 
\]

Additionally we will need the following lemma

**Lemma 4.5.** Let the initial value problem (2.1) satisfy the listed assumptions as well as \( F(t, u(t)) \in D(A) \), then

\[
\|a_{n-1} - b_{n-1}\|_X \leq CK^2 \|u_0\|_X + CK^2 \|Au_0\|_X + CDk^2 \\
+ CK^3 \sum_{j=1}^{n-1} \|AF(t_j, u_j)\|_X + CK \sum_{j=0}^{n-1} \|e_j\|_X.
\]

Similar to (4.2) we also have

\[
b_{n-1} = R_{1,1}^n(kA)u_0 + k^{-1}A^{-2}(R_{1,1}(kA) - I + kA) \\
\sum_{j=1}^{n-1} R_{1,1}^j(kA) (F(t_{n-j}, b_{n-j-1}) - F(t_{n-j-1}, v_{n-j-1})) \\
- A^{-1}(R_{1,1}(kA) - I) \sum_{j=1}^{n-1} R_{1,1}^j(kA)F(t_{n-j-1}, v_{n-j-1}) \\
- A^{-1}(R_{1,1}(kA) - I)F(t_{n-1}, v_{n-1}).
\]
Hence,

\[ a_{n-1} - b_{n-1} = \left( e^{-nkA} - R_{1,1}^n(kA) \right) u_0 + \sum_{j=1}^{n-1} \left( A^{-2} \left( e^{-j(k+1)A} - R_{1,1}^{j+1}(kA) \right) - A^{-2} \left( e^{-j(k+1)A} - R_{1,1}^{j}(kA) \right) \right) \]

\[ + k^{-1} A^{-2} (R_{1,1}(kA) - I + kA) \sum_{j=1}^{n-1} R_{1,1}^j(kA) \left( F(t_{n-j}, a_{n-j-1}) - F(t_{n-j}, b_{n-j-1}) \right) \]

\[ - k^{-1} A^{-2} (R_{1,1}(kA) - I + kA) \sum_{j=1}^{n-1} R_{1,1}^j(kA) \]

\[ (F(t_{n-j-1}, u_{n-j-1}) - F(t_{n-j-1}, v_{n-j-1})) \]

\[ - A^{-1} \sum_{j=1}^{n-1} \left( e^{-j(k+1)A} - R_{1,1}^{j+1}(kA) \right) - \left( e^{-j(k+1)A} - R_{1,1}^{j}(kA) \right) \right) F(t_{n-j-1}, u_{n-j-1}) \]

\[ - A^{-1} (R_{1,1}(kA) - I) \sum_{j=1}^{n-1} R_{1,1}^j(kA) \left( F(t_{n-j-1}, u_{n-j-1}) - F(t_{n-j-1}, v_{n-j-1}) \right) \]

\[ - A^{-1} e^{-kA} (R_{1,1}(kA) - I) F(t_{n-1}, u_{n-1}) \]

\[ - A^{-1} (R_{1,1}(kA) - I) \left( F(t_{n-1}, u_{n-1}) - F(t_{n-1}, v_{n-1}) \right) . \]
Thus,

\[ \|a_{n-1} - b_{n-1}\|_X \leq Ck^2 \|u_0\|_X + Ck^2 \sum_{j=1}^{n-1} \|F(t_{n-j}, a_{n-j-1}) - F(t_{n-j}, b_{n-j-1})\|_X + \]
\[ Ck \sum_{j=1}^{n-1} \|F(t_{n-j}, a_{n-j-1}) - F(t_{n-j}, b_{n-j-1})\|_X + \]
\[ Ck \sum_{j=1}^{n-1} \|F(t_{n-j-1}, a_{n-j-1}) - F(t_{n-j-1}, v_{n-j-1})\|_X + \]
\[ Ck^3 \sum_{j=1}^{n-1} \|F(t_{n-j-1}, u_{n-j-1})\|_X + \]
\[ Ck \sum_{j=1}^{n-1} \|F(t_{n-j-1}, a_{n-j-1}) - F(t_{n-j-1}, v_{n-j-1})\|_X + \]
\[ Ck^3 \|F(t_{n-1}, u_{n-1})\|_X + Ck \|F(t_{n-1}, u_{n-1}) - F(t_{n-1}, v_{n-1})\|_X \]
\leq Ck^2 \|u_0\|_X + CDk^2 + Ck^2 \sum_{j=1}^{n-1} \|a_{n-j-1} - u_{n-j-1}\|_X + \]
\[ Ck \sum_{j=1}^{n-1} \|a_{n-j-1} - b_{n-j-1}\|_X + Ck \sum_{j=0}^{n-1} \|e_{n-j-1}\|_X + Ck \sum_{j=0}^{n-1} \|u_{n-j-1}\|_X \]
\leq Ck^2 \|u_0\|_X + Ck^2 + Ck^2 \sum_{j=0}^{n-2} \|a_j - u_j\|_X + Ck \sum_{j=0}^{n-2} \|a_j - b_j\|_X + \]
\[ Ck \sum_{j=0}^{n-1} \|u_j\|_X + Ck \sum_{j=0}^{n-1} \|e_j\|_X \]

using (2.6) as well as (4.1). From (4.5) we obtain

\[ \|a_{n-1} - b_{n-1}\|_X \leq Ck^2 \|u_0\|_X + CDk^2 + Ck^3 \sum_{j=0}^{n-2} \|Au_j\|_X + Ck \sum_{j=0}^{n-2} \|a_j - b_j\|_X + \]
\[ + Ck^3 \sum_{j=0}^{n-1} \|u_j\|_X + Ck \sum_{j=0}^{n-1} \|e_j\|_X . \]

Applying Lemmas 4.3 and 4.4 yields

\[ \|a_{n-1} - b_{n-1}\|_X \leq Ck^2 \|u_0\|_X + Ck^2 \|Au_0\|_X + CDk^2 + Ck^3 \sum_{j=0}^{n-2} \|AF(t_j, u_j)\|_X + \]
\[ + Ck \sum_{j=0}^{n-2} \|a_j - b_j\|_X + Ck \sum_{j=0}^{n-1} \|e_j\|_X . \]
Here we can again apply Gronwall’s Lemma 4.1 with \( \varphi(t_n) = k \sum_{j=0}^{n-1} \|a_j - b_j\|_X \) and \( \Psi(t_n) = CDk^2 \|u_0\|_X + CK^2 \|Au_0\|_X + CDk^2 + CK^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X \) to obtain

\[
\varphi(t_{n-1}) = k \sum_{j=0}^{n-1} \|a_j - b_j\|_X \leq Ck \|a_0 - b_0\|_X + CK^2 \|u_0\|_X + CK^2 \|Au_0\|_X + CDk^2 \\
+ CK^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X + CK \sum_{j=0}^{n-1} \|e_j\|_X.
\]

Thus,

\[
\|a_{n-1} - b_{n-1}\|_X \leq Ck^2 \|u_0\|_X + CK^2 \|Au_0\|_X + CDk^2 \\
+ CK^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X + CK \sum_{j=0}^{n-1} \|e_j\|_X
\]

since

\[
\|a_0 - b_0\|_X = \left\| \left( e^{-kA} - R_{1,1}(kA) \right) u_0 - A^{-1} \left( e^{-kA} - R_{1,1}(kA) \right) F(t_0, u_0) \right\| \\
\leq CK^3 \|u_0\|_X + CK^3 \|F(t_0, u_0)\|_X \\
\leq CK^3 \|u_0\|_X + CDk^3.
\]

Now we can prove an error estimate for the difference between the semi-discrete scheme (3.3, 3.4) and the fully discrete scheme (3.7, 3.8), namely

**Theorem 4.6.** Let the initial value problem (2.1) satisfy the listed assumptions as well as \( F(t, u(t)) \in D(A) \). For the difference between the semi-discrete scheme (3.3, 3.4) and the fully discrete scheme (3.7, 3.8) the following error bound holds

\[
\|u_n - v_n\|_X \leq Ck^2 \|u_0\|_X + CK^2 \|Au_0\|_X + CDk^2 + CK^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_X
\]

uniformly on \( 0 \leq t_n \leq T \).

Let \( e_n = u_n - v_n \). Then

\[
e_n = a_{n-1} + \frac{1}{k} A^{-2} \left( e^{-kA} - I + kA \right) (F(t_n, a_{n-1}) - F(t_{n-1}, u_{n-1})) \\
- b_{n-1} - \frac{1}{k} A^{-2} (R_{1,1}(kA) - I + kA) (F(t_n, b_{n-1}) - F(t_{n-1}, v_{n-1})) \\
= a_{n-1} - b_{n-1} + \frac{1}{k} A^{-2} \left( e^{-kA} - R_{1,1}(kA) \right) (F(t_n, a_{n-1}) - F(t_{n-1}, u_{n-1})) \\
- \frac{1}{k} A^{-2} (R_{1,1}(kA) - I + kA) (F(t_n, b_{n-1}) - F(t_{n-1}, a_{n-1})) \\
- \frac{1}{k} A^{-2} (R_{1,1}(kA) - I + kA) (F(t_{n-1}, u_{n-1}) - F(t_{n-1}, v_{n-1}))
\]

(4.6)
Hence,
\[ \| e_n \|_X \leq \| a_{n-1} - b_{n-1} \|_X + C Dk^3 + C k^2 \| a_{n-1} - u_{n-1} \|_X + C k \| b_{n-1} - a_{n-1} \|_X + C k \| e_{n-1} \|_X. \]

Thus, using Lemmas 4.3, 4.4, 4.5 and equation (4.5)
\[ \| e_n \|_X \leq C k^2 \| u_0 \|_X + C k^2 \| Au_0 \|_X + C Dk^3 + C k^3 \sum_{j=0}^{n-1} \| Af(t_j, u_j) \|_X \]
\[ + C k \sum_{j=0}^{n-1} \| e_j \|_X + C Dk^3 + C k^2 \left( C k \| Au_{n-1} \|_X + C k \| u_{n-1} \|_X + C k \right) \]
\[ + C k \| e_{n-1} \|_X \]
\[ \leq C k^2 \| u_0 \|_X + C k^2 \| Au_0 \|_X + C Dk^3 + C k^3 \sum_{j=0}^{n-1} \| Af(t_j, u_j) \|_X \]
\[ + C k \sum_{j=0}^{n-1} \| e_j \|_X. \]

Lastly, we apply again Gronwall’s Lemma 4.1 with \( \varphi(t_n) = k \sum_{j=0}^{n} \| e_j \|_X \) and \( \Psi(t_n) = C k^2 \| u_0 \|_X + C k^2 \| Au_0 \|_X + C Dk^3 + C k^3 \sum_{j=0}^{n-1} \| Af(t_j, u_j) \|_X \) to obtain
\[ \| e_n \|_X \leq C k^2 \| u_0 \|_X + C k^2 \| Au_0 \|_X + C Dk^3 + C k^3 \sum_{j=0}^{n-1} \| Af(t_j, u_j) \|_X. \]

Overall we obtain the following theorem giving an error bound for the fully discrete scheme.

**Theorem 4.7.** If the listed assumptions are satisfied and \( F(t, u(t)) \in \mathcal{D}(A) \) as well as \( F \in C^2([0,T];L^1) \), then for the numerical solution the following error bound holds
\[ \| u(t_n) - v_n \|_X \leq C k^2 \max \left( \sup_{0 \leq \tau \leq T} \left\| F'(\xi, u(\xi)) \right\|_X, \sup_{0 \leq \tau \leq T} \left\| F(\tau, u(\tau)) \right\|_X, \right. \]
\[ \left. \| u_0 \|_X, \| Au_0 \|_X \right) + C Dk^3 \sum_{j=0}^{n-1} \| Af(t_j, u_j) \|_X \]
uniformly on \( 0 \leq t_n \leq T \). The constant \( C \) depends on \( T \), but is independent of \( n \) and \( k \).
Proof.

\[ \|u(t_n) - v_n\|_{X} \leq \|u(t_n) - u_n\|_{X} + \|u_n - v_n\|_{X} \]
\[ \leq Ck^2 \left( \sup_{0 \leq \tau \leq t_n} \left\| F'(\tau, u(\tau)) \right\|_{X} + \sup_{0 \leq \tau \leq t_n} \left\| F^{(2)}(\tau, u(\tau)) \right\|_{X} \right) \]
\[ + Ck^2 \|u_0\|_{X} + Ck^2 \|Au_0\|_{X} + CDk^2 + Ck^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{X} \]
\[ \leq Ck^2 \max \left( \sup_{0 \leq \tau \leq T} \left\| F'(\xi, u(\xi)) \right\|_{X}, \sup_{0 \leq \tau \leq T} \left\| F^{(2)}(\tau, u(\tau)) \right\|_{X} \right) \]
\[ \|u_0\|_{X}, \|Au_0\|_{X} \right) + Ck^3 \sum_{j=0}^{n-1} \|AF(t_j, u_j)\|_{X} + CDk^2 \]

by the preceding theorems. ■

V. NUMERICAL EXPERIMENTS

A. A Standard Example for Baseline Comparison

We consider the Brusselator in one spatial variable describing a chemical reaction with two components as given by the following system of PDE's, cf. [8]:

\[
\frac{\partial u}{\partial t} = A + u^2v - (B + 1)u + \alpha \frac{\partial^2 u}{\partial x^2} \\
\frac{\partial v}{\partial t} = Bu - u^2v + \alpha \frac{\partial^2 v}{\partial x^2}
\]

with \(0 \leq x \leq 1, A = 1, B = 3, \alpha = 1/50,\) and boundary conditions

\[
u(0, t) = u(1, t) = 1 \\
v(0, t) = v(1, t) = 3
\]

and initial conditions

\[
u(x, 0) = 1 + \sin(2\pi x) \\
v(x, 0) = 3.
\]

First, we verify that the assumptions are satisfied. Hence, let the Banach space \(X = L^1 \times L^1\)
and \(D_r = \left\{ w = \left( \begin{array}{c} u \\ v \end{array} \right) \in X : \|w\|_{\infty} \leq r \right\} \) with \(\|w\|_{\infty} = \max(\|u\|_{\infty}, \|v\|_{\infty})\) for \(r > 0\). Then, we have that \(D_r\) is locally closed in \(X\), \(F(t, w) = \left( \begin{array}{c} A - (B + 1)u + u^2v \\ Bu - u^2v \end{array} \right)\) is integrable, and \(F : [0, \infty) \times D_r \to X\) is continuous.Now, let \(M, R, \omega\) and \(T\) be given as in (2.4) and
let $x \in S_R$. Then, $E(t)x \in D$ by the maximum principle applied to the heat equation. Furthermore, since $u \in D_r$ implies that $\|u\|_\infty \leq r$, we also have that $\|u^2\|_\infty \leq r^2$. Hence, $u \in D_r$ implies $u^2 \in D_{r^2}$ and $v \in D_r$ implies $u^2v \in D_{r^3}$. Thus, we obtain that $F$ maps $[0,T] \times D$ back into $D$, where $s = \max(r,r^3)$. This yields that $d(x + hF(t,x);D_s) = 0$ and hence,

$$\liminf_{h \to 0^+} \frac{d(x + hF(t,x);D_s)}{h} = 0, \quad \forall (t,x) \in [0,T] \times D_s.$$ 

To show that the nonlinear function $F(t,w) = \begin{pmatrix} A - (B + 1)u + u^2v \\ Bu - u^2v \end{pmatrix}$ also satisfies Assumption 2.1 (Theorem 2.1), let $w_1, w_2 \in D_r$. Then we obtain

$$\|F(t,w_1) - F(s,w_2)\|_\mathcal{X} = \left\| \begin{pmatrix} A - (B + 1)u_1 + u_1^2v_1 \\ Bu_1 - u_1^2v_1 \end{pmatrix} - \begin{pmatrix} A - (B + 1)u_2 + u_2^2v_2 \\ Bu_2 - u_2^2v_2 \end{pmatrix} \right\|_\mathcal{X}$$

$$= \left\| \begin{pmatrix} -(B + 1)(u_1 - u_2) + u_1^2v_1 - u_1^2v_2 + u_1^2v_2 - u_2^2v_2 \\ B(u_1 - u_2) - (u_1^2v_1 - u_1^2v_2 + u_1^2v_2 - u_2^2v_2) \end{pmatrix} \right\|_\mathcal{X}$$

$$\leq \left\| \max(u_1 - u_2, v_1 - v_2) \begin{pmatrix} B + 1 + u_1^2 + (u_1 + u_2)v_2 \\ B + u_1^2 + (u_1 + u_2)v_2 \end{pmatrix} \right\|_\mathcal{X}$$

$$\leq L \|w_1 - w_2\|_\mathcal{X}.$$ 

For $w_1 \in D_s$, we have that $w_1^2 \in D_{s^2}$, hence $\|w_1\|_\infty \leq s$. Also, $w_1 \in D_r$ implies that $\|w_1\|_\infty \leq r$ as well as $\|v_1\|_\infty \leq r$. The same applies to $w_2$; i.e., $u_2$ and $v_2$. Hence, $\|u_1v_2\|_\infty \leq r^2$ as well as $\|u_2v_2\|_\infty \leq r^2$. Therefore, $\|B + 1 + u_1^2 + (u_1 + u_2)v_2\|_\mathcal{X} \leq L_1 \leq L$ and $\|B + u_1^2 + (u_1 + u_2)v_2\|_\mathcal{X} \leq L_2 \leq L$, where $L = \max(L_1, L_2)$, which depends on $r$.

We integrate the problem for $0 \leq t \leq 10$ in order to demonstrate the performance of the scheme. Figure 1 contains a solution profile.

Table I shows the observed $\ell_2$-errors and rates for this problem. As expected the rate of convergence is 2.

Table II shows an observed timing comparison between ETD-CN and the standard Crank-Nicolson and BDF-2 schemes. Here, for the Crank-Nicolson and BDF-2 schemes we employ a modified Newton’s method as in the previous paragraph. The data show how significant the improvement can be when using the ETD version of the Crank-Nicolson scheme as compared
TABLE I. Example A. Numerical errors ($\ell_2$) and rates using ETD-CN for the Brusselator equation.

<table>
<thead>
<tr>
<th>$h$</th>
<th>$k = h$</th>
<th>Error ETD-CN</th>
<th>Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.1</td>
<td>$3.0 \times 10^{-3}$</td>
<td>1.9499</td>
</tr>
<tr>
<td>0.05</td>
<td>0.05</td>
<td>$7.7718 \times 10^{-4}$</td>
<td>1.9763</td>
</tr>
<tr>
<td>0.025</td>
<td>0.025</td>
<td>$1.9751 \times 10^{-4}$</td>
<td>1.9867</td>
</tr>
<tr>
<td>0.0125</td>
<td>0.0125</td>
<td>$4.9833 \times 10^{-5}$</td>
<td>1.9974</td>
</tr>
<tr>
<td>0.00625</td>
<td>0.00625</td>
<td>$1.2481 \times 10^{-5}$</td>
<td>2.0179</td>
</tr>
<tr>
<td>0.003125</td>
<td>0.003125</td>
<td>$3.0816 \times 10^{-6}$</td>
<td></td>
</tr>
</tbody>
</table>

TABLE II. Numerical errors ($\ell_2$) and CPU-time (sec) using ETD-CN, Crank-Nicolson, and the second order Backward Differentiation Formula (BDF-2) for Brusselator equation.

<table>
<thead>
<tr>
<th>$h$</th>
<th>$k = h$</th>
<th>Error ETD-CN</th>
<th>CPU</th>
<th>Error CN</th>
<th>CPU</th>
<th>Error BDF-2</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.1</td>
<td>$3.0 \times 10^{-3}$</td>
<td>0.016</td>
<td>$3.1 \times 10^{-3}$</td>
<td>0.078</td>
<td>$3.3 \times 10^{-3}$</td>
<td>0.062</td>
</tr>
<tr>
<td>0.05</td>
<td>0.05</td>
<td>$7.77 \times 10^{-4}$</td>
<td>0.031</td>
<td>$7.96 \times 10^{-4}$</td>
<td>0.297</td>
<td>$1.0 \times 10^{-3}$</td>
<td>0.313</td>
</tr>
<tr>
<td>0.025</td>
<td>0.025</td>
<td>$1.98 \times 10^{-4}$</td>
<td>0.078</td>
<td>$1.96 \times 10^{-4}$</td>
<td>2.156</td>
<td>$2.53 \times 10^{-4}$</td>
<td>2.204</td>
</tr>
<tr>
<td>0.0125</td>
<td>0.0125</td>
<td>$4.98 \times 10^{-5}$</td>
<td>0.531</td>
<td>$4.91 \times 10^{-5}$</td>
<td>22.078</td>
<td>$6.34 \times 10^{-5}$</td>
<td>22.437</td>
</tr>
</tbody>
</table>

to the two standard schemes on this well-known test case. However, if the Crank-Nicolson and BDF(2) schemes are applied in a linearly implicit manner, they will use less CPU time.
but their convergence rates will seriously deteriorate. Our aim is to keep the convergence order of all the test examples the same (second order).

B. A Chemotaxis Example

We consider a system of PDEs which describes chemotactic behavior of bacteria, especially 

\[ E. \text{coli} \text{ and } S. \text{typhimurium}, \]

given by

\[
\frac{\partial n}{\partial t} = D_n \nabla^2 n - \alpha \nabla \left( \frac{n}{(1 + c)^2} \nabla c \right) + \rho n \left( \delta \frac{s^2}{1 + s^2} - n \right)
\]

\[
\frac{\partial c}{\partial t} = D_c \nabla^2 c + \beta s \frac{n^2}{\gamma + n^2} - nc
\]

\[
\frac{\partial s}{\partial t} = D_s \nabla^2 s - \kappa n \frac{s^2}{\delta + s^2},
\]

where \( n \) denotes the bacterial cell density, \( c \) the aspartate concentration, and \( s \) the succinate concentration. Here, \( D_n, D_c, D_s \) are the diffusion coefficient for cells, chemoattractant, and succinate, respectively; \( \alpha \) is the chemotaxis coefficient, \( \beta \) the production of chemoattractant, \( \gamma \) the saturation of production of chemoattractant, \( \delta \) the carrying capacity or yield coefficient, \( \rho \) the growth rate for cells, and \( \kappa \) the consumption of food, which are experimentally determined parameters.

The dimensionless parameters we use are identical to those contained in Murray [21] or Tyson [27], \( D_n = 0.25, D_c = 1.0, D_s = 1.0, \alpha = 7.0, \beta = 10.0, \gamma = 250.0, \delta = 10.0, \rho = 0.1, \kappa = 0 \). The domain \( \Omega \) is assumed to be a square of side length 20 cm.

In this problem the initial data is often discontinuous, and previous treatments [21, 27] have used some kind of mollifying procedure as a pretreatment of the initial function; however, the ETD-CN scheme with initial damping naturally handles the nonsmooth data case without modification. For damping we use an Exponential Time Differencing Version of the Backward Euler Scheme (ETD-BE). The initial data in this example is a jump function:

\[
\begin{align*}
n(x,y,0) &= \begin{cases} 
2 & \text{if } d \leq r \\
0 & \text{otherwise} 
\end{cases} \\
c(x,y,0) &= 0 \\
s(x,y,0) &= 5,
\end{align*}
\]

where \( d \) is the euclidean distance to the center \((x_0, y_0) = (10, 10)\) and \( r \) is the width of the inoculum of bacteria; i.e., initially succinate is distributed uniformly throughout the medium and an inoculum of bacteria is put at the center of the medium with radius \( r \). For \( E. \text{coli} \) a very low density bacterial population forms, which then spreads outwards from the

---

**FINAL VERSION**  March 14, 2011, 7:27am
initial inoculum. Within this bacterial population high density rings of bacteria are seen. For *S. typhimurium* a swarm ring (high density ring of energetically agile bacteria) forms and disperses away from the initial inoculum. The bacterial density in this swarm ring increases until a special point, when it becomes unstable and a percentage of the bacteria are left behind as aggregates which remain full of energetically agile bacteria for a short period of time and then disband as the bacteria combines again with the swarm ring. A clump of bacteria is left behind in the aggregates original location; this is non-motile.

We see concentric rings that are formed as the bacteria moves outward. The domain is assumed to be large enough such that the bacteria never reaches the boundary. We assume Neumann boundary conditions on the boundary $\partial \Omega$:

\[
\frac{\partial}{\partial \nu} n(x, y, t) = 0
\]
\[
\frac{\partial}{\partial \nu} c(x, y, t) = 0
\]
\[
\frac{\partial}{\partial \nu} s(x, y, t) = 0.
\]
VI. APPLICATION TO FINANCE

In this section we shall demonstrate the performance of the proposed scheme by implementing it on a nonlinear Black–Scholes (BS) equation. We take the model of Hoggard, Whalley, and Wilmott [11], which is based on Leland [16]. It is given by

\[ V_t + \frac{1}{2} \sigma^2 S^2 V_{SS} + \rho S V_S - \rho V = \epsilon S^2 |V_{SS}| \]  

(6.1)

with

\[ \epsilon = \kappa \sigma \sqrt{\frac{2}{\pi \delta \tau}} \]

and terminal condition

\[ V(S, \tau_0) = V_0(S), \quad S \geq 0, \]

where \( S \) is the price of the underlying asset, \( \rho \) the risk-free interest rate, \( \sigma \) the asset volatility, \( \kappa \) a proportionality constant, and \( V(S, \tau) \) the price of the option written on \( S \), respectively. The portfolio is considered to be revised every \( \delta \tau \) where \( \delta \tau \) is a fixed time step, cf. [13].

Equation (6.1) is one of the most recent models for the pricing of transaction costs in quantitative finance. In the case that \( \epsilon \) is zero, the analysis of which assumes a perfect market with hedging taking place continuously (\( \delta \tau \rightarrow 0 \)), the standard BS equation arises [1]. Leland [16] included transaction costs proportional to the value of shares traded into the BS equation. In his model it is assumed that hedging takes place at discrete time intervals and additionally, that the resulting option price is a convex function of the asset price, i.e. that the “Gamma” is of the same sign for all \( S \) and \( t \). Hoggard et al. [11] relaxed the assumptions and derived the HWW equation. Imai and Ishimura [13] proved the existence of solutions for the case \( \epsilon \leq \sigma^2/2 \).

In the next subsections we present several numerical examples based on HWW, each with different initial or boundary assumptions.

A. A European Call Option with Nonlinear Transaction Costs

For a European Call option we have

\[ V_0(S) = \max(0, S - E), \]

with asset price \( S \), exercise price \( E \), and boundary conditions

\[ V(0, \tau) = 0, \quad \tau_0 \geq \tau \geq 0, \quad V(S, \tau) \propto S - E e^{\rho(\tau - \tau_0)}. \]
i.e.,
\[ \lim_{S \to \infty} \frac{V(S, \tau)}{S - E e^{\rho(\tau - \tau_0)}} = 1, \]
uniformly for \( 0 \leq \tau \leq \tau_0 \).

To obtain a forward parabolic problem, we use the same transformations as D"uring et al. [5], namely
\[ x = \log \left( \frac{S}{E} \right), \quad t(\tau) = \frac{1}{2} \sigma^2 (\tau_0 - \tau), \quad u = e^{-x} \frac{V}{E}. \]

Then (6.1) is transformed into
\[ u_t = u_{xx} + \left( 1 + \frac{2\rho}{\sigma^2} \right) u_x + \frac{2}{\sigma^2} \epsilon |u_{xx} + u_x| \quad (6.2) \]
with initial condition
\[ u(x, 0) = \max(0, 1 - e^{-x}) \]
and boundary conditions
\[ u(x, t) = 0 \quad \text{as} \quad x \to -\infty \quad u(x, t) \propto 1 \quad \text{as} \quad x \to \infty, x \in \mathbb{R}. \]

For the computation we need to replace \( \mathbb{R} \) by \([-R, R]\) where \( R > 0 \) is large enough to cover the range of interest for the asset price. We denote the space step by \( h \), the time step by \( k \), and the approximate solution of (6.2) at \( x_i \) at time \( t_n = nk \) by \( u^n_i \). For simplicity we generate an equidistant mesh in the spatial variable. Then the boundary conditions are
\[ u(x_{-N}, t) = 0 \quad u(x_N, t) = 1 - e^{-x_N - \frac{2\rho}{\sigma^2} t}. \]

Using a straightforward centered differences approach in the spatial variable, we computed with the ETD-CN scheme using the HWW equation model with nonlinear transaction costs. We now compare the HWW model approximated through ETD-CN to a more complex model proposed by Barles and Soner [2], which D"uring et al. use in their numerical experiments using a compact finite difference scheme called R3C [5]. This model incorporates transaction cost via a nonlinear volatility, as follows:
\[ V_\tau + \frac{1}{2} \sigma (V_{SS})^2 S^2 V_{SS} + \rho SV_S - \rho V = 0, \quad (6.3) \]
where
\[ \sigma (V_{SS})^2 = \sigma_0^2 \left( 1 + \Psi(\exp(\rho(\tau_0 - \tau))a^2 S^2 V_{SS}) \right) \]
with transaction cost parameter $a = \mu \sqrt{\gamma N}$ with risk aversion factor $\gamma$ and $N$ being the number of options sold. The function $\Psi$ is the solution to the nonlinear initial-value problem

$$\Psi'(A) = \frac{\Psi(A) + 1}{2 \sqrt{A \Psi(A)} - A}, \quad A \neq 0$$

with initial condition $\Psi(0) = 0$.

For the comparison of the numerical schemes we choose the same parameters as Dürring et al. in [5], namely

$$\rho = 0.1, \quad \sigma = 0.2, \quad E = 100, \quad \epsilon = 0, \quad t_{end} = 0.04 = 2 \text{ years}.$$  

Dürring et al. solve (6.3) using the compact finite difference scheme R3C, whereas we solve (6.1) with ETD-CN. The solution at time $t = 0.02 \approx 1$ year is plotted in Figure 3 for the R3C scheme for values $a = 0, 0.01, \text{ and } 0.02$ and for the ETD-CN scheme for values $\epsilon = 0, 0.0075, \text{ and } 0.015$. Very similar numerical approximations result.

![Figure 3](image)

(a) Barles & Soner model & R3C scheme.  
(b) HWW model & ETD-CN.

FIG. 3. Solution at $t = 0.02 \approx 1$ year. Plotted are the option prices for different values of the transaction costs, with pay-off.

Figure 4 shows a simultaneous plot of the solutions for the Barles and Soner model with R3C and the HWW model with ETD-CN at $t = 0.02$. Noting that essentially no difference can be seen, we conclude that the two approaches yield the same solutions. However, timing experiments show that the HWW/ETD-CN approach is more than twice as fast as the Barles & Soner/R3C version. The timing differences may be due to the more complex model of Barles and Soner.

To show that the proposed scheme is second order accurate we calculated a reference solution using a forward Euler scheme on a very fine mesh. Here we choose the same parameters as Imai et al. in [13], namely $\rho = 0.1, \sigma = 0.4, t = 0.04 = \frac{1}{2} \text{ year}, E = 45, \epsilon = 0.02, \text{ and } R = 2$. Table III shows the errors in the infinity-norm and the convergence rates, where
we keep the ratio $\mu = k/h$ fixed. The rates show that the scheme is indeed second order accurate.

Figure 5 shows the solution and the difference between the nonlinear and linear models at time $t = 0.04 \approx 1/2$ year for $\sigma = 0.4$. We see that the difference is not symmetric and that it is maximal near the exercise price $E$. After half a year the maximum difference is at approximately $S = 45$ which is the exercise price of the option. The linear Black–Scholes price is about 4.1233 whereas the nonlinear price is about 4.53 using a transaction cost parameter of $\epsilon = 0.02$. Thus, the nonlinear price is approximately 9.9% higher than the linear Black–Scholes price.

Figure 6 shows a double logarithmic plot of the errors.
TABLE III. $\ell_\infty$-errors and rates of the ETD-CN scheme on the HWW model with the parameters of Figure 5.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$k$</th>
<th>Error</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.4</td>
<td>$8 \times 10^{-3}$</td>
<td>1.5153</td>
<td>2.1312</td>
</tr>
<tr>
<td>10</td>
<td>0.2</td>
<td>$4 \times 10^{-3}$</td>
<td>0.3459</td>
<td>2.1263</td>
</tr>
<tr>
<td>20</td>
<td>0.1</td>
<td>$2 \times 10^{-3}$</td>
<td>0.0792</td>
<td>2.0289</td>
</tr>
<tr>
<td>40</td>
<td>0.05</td>
<td>$1 \times 10^{-3}$</td>
<td>0.0194</td>
<td>2.0188</td>
</tr>
<tr>
<td>80</td>
<td>0.0250</td>
<td>$5 \times 10^{-4}$</td>
<td>0.0048</td>
<td>2.0293</td>
</tr>
<tr>
<td>160</td>
<td>0.0125</td>
<td>$2.5 \times 10^{-4}$</td>
<td>0.0012</td>
<td>2.0622</td>
</tr>
<tr>
<td>320</td>
<td>0.00625</td>
<td>$1.25 \times 10^{-4}$</td>
<td>0.00028</td>
<td></td>
</tr>
</tbody>
</table>

FIG. 6. (L) Double logarithmic plot of error versus space step $h$, indicating second order convergence. Efficiency plot (R), CPU time (sec) versus error. Parameters are those of Figure 5.

The most common option price sensitivities are the first and second derivatives with respect to the price of the underlying asset. They are called “Delta” and “Gamma”, respectively. As price sensitivities are a striking measure of risk, they are important features in risk management. These functions are challenging to compute numerically. Figure 7 shows the errors in the Greeks of the numerical solution calculated using the same parameters as in Figure 5 using HWW/ETD-CN (and for the linear case $\epsilon = 0$) with centered differences as approximations for the first and second derivative.

B. Butterfly Spread

A Butterfly Spread is a combination of three options with three strike prices, in which one contract is purchased with two outside strike prices and two contracts are sold at the middle
strike price. The payoff function at expiry for a Butterfly Spread is therefore given by

\[ V(S, \tau_0) = V_0(S) = \max(0, S - E_1) - 2 \max(0, S - E_2) + \max(0, S - E_3) \quad (6.4) \]

for \( 0 \leq S \leq S_{\text{max}} \) where \( E_1, E_2, \) and \( E_3 \) are the strike prices that satisfy \( E_1 < E_2 < E_3 \) and \( E_2 = (E_1 + E_3)/2 \). The boundary conditions are homogeneous, i.e.

\[ V(0, \tau) = V(S_{\text{max}}, \tau) = 0, \quad \tau_0 \geq \tau \geq 0. \quad (6.5) \]

The initial data has corners at the three strike prices \( E_1, E_2, \) and \( E_3 \), hence its Delta has three jump discontinuities. The behavior of Delta at expiry looks like

\[
\lim_{\tau \to \tau_0^-} \frac{\partial V}{\partial S} = \begin{cases} 
0 & \text{for } 0 \leq S < E_1 \\
1 & \text{for } E_1 \leq S < E_2 \\
-1 & \text{for } E_2 \leq S < E_3 \\
0 & \text{for } S \geq E_3.
\end{cases}
\]

We consider the following model:

\[ V_\tau + \frac{1}{2} \sigma^2 S^2 V_{SS} + \rho S V_S - \rho V = \epsilon S^2 |V_{SS}| \quad 0 \leq S \leq 100, \quad 1 \geq \tau \geq 0 \]

with final condition (6.4) and homogeneous boundary conditions (6.5). We use the transformation \( t = \tau_0 - \tau \) to obtain a forward parabolic problem and choose the following parameters (as in Khaliq et al. [15]):

\[ \rho = 0.1, \quad \sigma = 0.5 \quad t = 1 \quad E_1 = 40 \quad E_2 = 50 \quad E_3 = 60. \quad (6.6) \]
We choose the high volatility of $\sigma = 0.5$ to show that the method is stable also for large values of $\sigma$.

Figure 8 shows the solution at $t = 1$ using $\epsilon = 0$ and $\epsilon = 0.02$ as cost parameters. A time evolution profile using ETD-CN with and without smoothing steps is shown in Figure 9. Without initial smoothing there is significant error near the three strike prices $E_1, E_2,$ and $E_3$ due to amplification of the higher frequency components near the corners in the initial conditions. With at least two steps of initial damping these oscillations are eliminated; we have used four steps due to slightly better performance.

![Figure 8](image1.png)

(a) ETD-CN  
(b) ETD-CN after 4 steps of ETD-BE

FIG. 8. Solution of the Butterfly Spread problem at $t = 1$ using $\epsilon = 0$ (linear case) and $\epsilon = 0.02$ as cost parameters (6.6).

![Figure 9](image2.png)

(a) ETD-CN  
(b) ETD-CN after 4 steps of ETD-BE

FIG. 9. Time evolution profile for the Butterfly Spread using the nonlinear HWW model with ETD-CN and parameters (6.6).

Figures 10 and 11 show time evolution profiles of Delta and Gamma, respectively, for the Butterfly option. We see oscillations near the strike prices in the undamped scheme which
are eliminated using four steps of initial smoothing. The graphs were generated using 80 grid points for the space, i.e. $\Delta S = 1.25$, $\Delta t = 0.1$ and the parameters (6.6).

FIG. 10. Butterfly Spread Delta for nonlinear HWW model with ETD-CN using parameters (6.6).

FIG. 11. Butterfly Spread Gamma for nonlinear HWW model with ETD-CN using parameters (6.6).

C. Digital Call Option

The Digital Call also has a nonsmooth payoff function like the Butterfly Spread. For the Butterfly Spread the payoff is continuous, while it is discontinuous for the Digital Call. Additionally, the Butterfly Spread is homogeneous at the boundary, whereas the Digital Call problem has one boundary condition that is time-dependent. The PDE for a Digital Call is
given by (6.1) with final condition
\[
\lim_{\tau \to \tau_0} V(S, \tau) = \begin{cases} 
A & \text{for } S > E \\
0 & \text{for } S < E \\
0 & \text{for } S \leq S_{max} \leq S_{max} 
\end{cases}
\] (6.7)
which is also called “cash-or-nothing”. Here, \( A > 0 \) is the payoff amount at expiry. We average the payoff as
\[
\lim_{\tau \to \tau_0} V(S, \tau) = \begin{cases} 
A & \text{for } S > E \\
\frac{A}{2} & \text{for } S = E \\
0 & \text{for } S < E. 
\end{cases}
\] (6.8)
The boundary conditions are given as
\[
V(0, \tau) = 0 \quad \tau_0 \geq \tau \geq 0 \\
V(S, \tau) \approx Ae^{-\rho(\tau_0 - \tau)} \quad \text{as } S \to \infty,
\] (6.9)
since the asset remains zero if \( S = 0 \) and therefore the payoff will be zero and the option is almost certain to pay off \( A \) if \( S \) is large. We employ the following PDE model:
\[
V_\tau + \frac{1}{2} \sigma^2 S^2 V_{SS} + \rho S V_S - \rho V = \epsilon S^2 |V_{SS}| \quad 0 \leq S \leq 80, \quad 0.5 \geq \tau \geq 0, (6.10)
\] with final condition (6.8) and boundary conditions given by (6.9). We use the transformation \( t = \tau_0 - \tau \) to obtain a forward parabolic problem and choose the following parameters [15]:
\[
\rho = 0.05, \quad \sigma = 0.3, \quad t_{end} = 0.5, \quad E = 40, (6.11)
\] and \( \epsilon = \sigma^2/2 = 0.045 \).

Figure 12 shows the solution at \( t = 0.5 \) using \( \epsilon = 0 \) and \( \epsilon = 0.045 \) as cost parameters. A time evolution profile using ETD-CN with and without initial smoothing steps is shown in Figure 13.

Figures 14 and 15 show time evolution profiles of Delta and Gamma for the Digital Call option.

The graphs were generated using 480 grid points for the space, i.e. \( \Delta S = 0.167 \) and \( \Delta t = 0.05 \) and the parameters (6.11).
FIG. 12. Solution of Digital Call problem (6.7) – (6.10) at \( t = 0.5 \) using ETD-CN, \( \epsilon = 0 \) and \( \epsilon = 0.045 \) as cost parameters.

FIG. 13. Time evolution profile for the Digital Call (6.7) – (6.10) using ETD-CN, as in Figure 12.

VII. CONCLUSION

We derive a new fully discrete Exponential Time Differencing Runge-Kutta method followed by a (1,1)-diagonal Padé scheme to solve nonlinear parabolic partial differential equations. Convergence of the new scheme is proved for the semilinear case and demonstrate its convergence with several examples. A comparison the new scheme ETD-CN to other standard second order codes like the Crank-Nicolson and BDF-2 schemes shows the effectiveness of the new algorithm. ETD-CN is faster due to the fact that it does not have to solve nonlinear systems in each time step, yet it remains second order accurate.

In applications one often encounters nonsmooth initial data, which in most well-known second order codes inflicts oscillations if not treated carefully. Here, we demonstrate that between two and four steps of initial damping suffices to restore the good numerical properties of ETD-CN. In an application to finance we chose the Hoggard, Whalley, and Wilmott[11] equation, which is a nonlinear model, to evaluate the price of several options. Due to the nonlinear transaction cost term and nonsmooth initial conditions, this equation is difficult to accurately resolve. We show numerically that the ETD-CN scheme remains second order accurate even with these challenging conditions.

The new scheme is comparable to other well known second order schemes in accuracy, yet is more effective with regard to CPU time.

REFERENCES


FINAL VERSION March 14, 2011, 7:27am


