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A Nonstandard Finite Difference Scheme for Convection-Diffusion Equations having Constant Coefficients

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Abstract

In this note we derive, using the subequation method, a new nonstandard finite difference scheme (NSFD) for a class of convection-diffusion equations having constant coefficients. Despite the fact that this scheme has nonlinear denominator functions of the step sizes (even for linear PDEs), it has a couple of favourable properties: it is explicit and due to its construction it reproduces important properties of the solution of the parabolic PDE. This proposed method conserves, by construction, the positivity of the solution and hence it is perfectly suited for solving for example air pollution problems or the Black–Scholes equation for the valuation of standard options, since it avoids negative values for the calculated prices. Finally, we illustrate the usefulness of this newly proposed method on a classical benchmark example from the literature.

Key words: convection-diffusion equation, positivity, nonstandard finite difference method, subequation method, option pricing, air pollution

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1 Introduction

In the process of modelling and simulation of physical and other phenomena, it is desirable that numerical quantities reflect the original system behaviour, e.g. in electrical engineering, where the charge transport in semiconductor devices is usually described by a convection-diffusion equation. Here the charge transport is described in terms of charge carrier densities, which should be non-negative. Similar reasoning holds for the simulation of the pollutant density in air pollution problems [1]. Also, in financial applications, e.g. the computation of the fair price of an option, one is interested in numerical methods that guarantees the positivity of the solution.

Hence, it is of tremendous importance to construct such *positivity preserving schemes* [2,3] that avoid unrealistic negative values for the solution and, as a side-effect, are stable with respect to the maximum norm. One possibility are so-called *nonstandard finite difference (NSFD) methods*. These methods are tailor made special schemes for the numerical integration of differential equations in order to preserve certain properties (positivity, asymptotic behaviour, etc.) of the analytic solution on the discrete computational grid. The general basic rules to construct NSFDs [4,5] are the following:

- The orders of the discrete derivatives should be equal to the orders of the corresponding derivatives appearing in the differential equations.
- Discrete representations for derivatives must, in general, have nontrivial denominator functions.
- Nonlinear terms should, in general, be replaced by nonlocal discrete representations.
- Special conditions that hold for the differential equation and/or its solutions should also hold for the difference equation model and/or its solutions.

Here we will demonstrate how to construct an explicit NSFD scheme for a general convection-diffusion type PDE having constant coefficients of the form

$$u_\tau + b u_x = a u_{xx} - c u, \tag{1}$$

by using the *subequation method* in the context of the NSFD scheme methodology. The use of subequations and their discretizations form the basis for these constructions of the full PDE.

The basic idea is to start from an explicit upwind discretization, construct suitable denominator functions and then develop a strategy for choosing the time step appropriately. In general, the NSFD methodology gives a functional relation between the space step Δx and the time step Δt . This follows immediately from the positivity requirement. Thus, there will be a time step limitation for a given Δx , but usually it will be less restrictive than for other standard

explicit finite difference schemes. Here we focus on the financial application, especially the option pricing problem, but also explain an application in air pollution simulation.

This work is organized as follows: first we introduce in §2 the Black–Scholes equation for pricing European and American options, recall the standard transformation to a forward-in-time heat equation which is of the form (1). Next, in §3 we describe briefly the PDEs appearing in air pollution simulations, which is another application field: In §4 we present the *subequation method* which is the basic tool in deriving the NSFD scheme. Here, it will turn out to be necessary to distinguish between the two cases with and without a reaction rate. Afterwards we analyze in §5 the properties of the resulting numerical scheme by the modified equation technique. Finally, we illustrate in §6 the accuracy and efficiency of the new method with a numerical textbook example and compare it to classical finite difference schemes.

2 Option Pricing

The famous Black–Scholes equation is an effective model for option pricing. It was named after the pioneers Black, Scholes and Merton who suggested it 1973 [6,7] and received in 1997 the Nobel Prize in Economics for their discovery [8]. Mathematically it is a final value problem for a backward-in-time second order parabolic equation. A concise derivation of the Black–Scholes equation can be found in [9].

An option is a contract that admits the owner the right (not the duty) to buy (*‘call option’*) or to sell (*‘put option’*) an asset (typically a stock or a parcel of shares of a company) for a prespecified price K (*‘strike price’*) by the date T to receive some payoffs. The basic problem here is to specify a fair price to charge for permitting these rights. A closely related question is how to hedge the risks that arises when selling these options. ‘European’ options can only be exercised at the expiration date T . For ‘American’ options exercise is permitted at any time until the expiry date. The notion European or American are not meant geographically, they just declare the type of option.

In general, closed–form solutions do not exist (especially for American options) and the solution has to be computed numerically. The standard approach for solving the Black–Scholes equation for pricing options consists in transforming the original equation to a convection-diffusion equation posed on a semi-unbounded domain [10,9]. Often finite differences are used to discretize this convection-diffusion equation and *artificial boundary conditions* (ABCs) [11] are introduced in order to confine the computational domain appropriately and retain the accuracy and stability properties of the underlying scheme.

Next we present one standard example, the European put, that will lead us to a heat equation that is of the form (1).

2.1 The European Call Option

Here we focus on *European Call options*; the treatment of *European Put options* is analogous. The *value of a Call option* is denoted by V and depends on the current market price of the underlying asset, S , (the letter ' S ' symbolizes *stocks*) and the calendar time t : $V = V(S, t)$. The *Black–Scholes equation* is a backward–in–time parabolic equation

$$\frac{\partial V}{\partial t} + \frac{\sigma^2}{2} S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0, \quad S > 0, \quad 0 \leq t < T, \quad (2)$$

where σ denotes the annual *volatility* of the asset price, r the risk–free interest rate and T is the *expiry date* ($t = 0$ means 'today').

The *terminal condition* ('payoff condition') at the expiry $t = T$ reads

$$V(S, T) = (S - K)^+, \quad S \geq 0, \quad (3)$$

with the notation $f^+ = \max(f, 0)$. Here $K > 0$ denotes the previously agreed *exercise price* or 'strike', of the contract.

The 'spatial' or asset–price *boundary conditions* for European Call options at $S = 0$, and $S \rightarrow \infty$ are

$$V(0, t) = 0, \quad 0 \leq t \leq T, \quad (4a)$$

$$V(S, t) \sim S - K e^{-r(T-t)} \quad \text{as } S \rightarrow \infty, \quad 0 \leq t \leq T. \quad (4b)$$

i.e. at $S = 0$ the option is worthless. Correspondingly, we have for a European Put the terminal condition

$$V(S, T) = (K - S)^+, \quad S \geq 0, \quad (5)$$

and the boundary conditions

$$V(0, t) = 0, \quad \text{as } S \rightarrow \infty, \quad 0 \leq t \leq T, \quad (6a)$$

$$V(S, t) = K e^{-r(T-t)} - S \quad \text{for } S \approx 0, \quad 0 \leq t \leq T. \quad (6b)$$

The focus of this paper is the numerical solution of the problem, which is achieved by initially analytically approaching the solution for the European call by transforming (2) with (3), (4) into a forward-in-time parabolic problem. In the following sections both a classical and a NSFD scheme will be specified and used to solve the transformed problem.

2.2 The Transformation to the Heat Equation

We now review how to transform (2) into a pure diffusion equation (cf. [9, § 5.4]). It is convenient to apply time reversal and transform (2) to a *forward-in-time equation* by the change $t = T - 2\tau/\sigma^2$. The new time variable τ stands for (up to the scaling by $\sigma^2/2$) the *remaining life time* of the option. We denote the new variables by:

$$\tilde{V}(S, \tau) = V(S, t) = V\left(S, T - \frac{2\tau}{\sigma^2}\right), \quad \tilde{r} = \frac{2}{\sigma^2}r, \quad \tilde{T} = \frac{\sigma^2}{2}T.$$

The resulting forward-in-time equation then reads:

$$\frac{\partial \tilde{V}}{\partial \tau} = S^2 \frac{\partial^2 \tilde{V}}{\partial S^2} + \tilde{r}S \frac{\partial \tilde{V}}{\partial S} - \tilde{r} \tilde{V}, \quad S > 0, \quad 0 \leq \tau < \tilde{T}, \quad (7)$$

which is supplied, in case of a European call, with the initial condition

$$\tilde{V}(S, 0) = (S - K)^+, \quad S \geq 0, \quad (8)$$

and the boundary conditions

$$\tilde{V}(0, \tau) = 0, \quad 0 \leq \tau \leq \tilde{T}, \quad (9)$$

$$\tilde{V}(S, \tau) \sim S - Ke^{-r(2\tau/\sigma^2)} \quad \text{as } S \rightarrow \infty, \quad 0 \leq \tau \leq \tilde{T}. \quad (10)$$

The right hand side of (7) is the well-known *Euler's differential equation expression* and therefore it is standard practice (cf. [10]) to transform (7) to the heat equation. To do so, we let $\alpha = -(\tilde{r} - 1)/2$, $\lambda = -\alpha^2 - \tilde{r}$, and use the change of variables

$$S = Ke^x, \quad \tilde{V}(S, \tau) = Ke^{\alpha x + \lambda \tau} v(x, \tau).$$

Then problem (7)–(10) is equivalent to the initial boundary value problem for the heat equation:

$$\frac{\partial v}{\partial \tau} = \frac{\partial^2 v}{\partial x^2}, \quad x \in \mathbb{R}, \quad 0 \leq \tau < \tilde{T}, \quad (11)$$

with the initial condition

$$v(x, 0) = \left(e^{\frac{1}{2}(\tilde{r}+1)x} - e^{\frac{1}{2}(\tilde{r}-1)x}\right)^+, \quad x \in \mathbb{R}, \quad (12)$$

and with the asymptotic boundary conditions for $0 \leq \tau \leq \tilde{T}$:

$$v(x, \tau) = 0 \quad \text{for } x \rightarrow -\infty, \quad (13)$$

$$v(x, \tau) = \exp\left(\frac{\tilde{r}+1}{2}x + \frac{(\tilde{r}+1)^2}{4}\tau\right) \quad \text{for } x \rightarrow \infty. \quad (14)$$

The problem how to appropriately confine the spatial domain for solving the whole space problem (11) posed on $x \in \mathbb{R}$ by (discrete) artificial boundary conditions that preserve the stability, accuracy and computational effort of the interior scheme, was discussed concisely in [11]. Thus, in the following work we will restrict ourselves to the task of constructing a suitable interior NSFD method.

Next, we briefly sketch another application from environmental simulations that can be written as a convection-diffusion equation in 1D. Also here it is essential that the computed concentrations of the pollutants remain positive.

3 Air Pollution Simulation

The process of pollutant transport and diffusion in the atmosphere (and also in water) is described by the following *advection–diffusion equation* [12]:

$$\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} + v \frac{\partial \varphi}{\partial y} + (w - w_g) \frac{\partial \varphi}{\partial z} - \mu \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right) - \frac{\partial}{\partial z} \left(\nu \frac{\partial \varphi}{\partial z} \right) + \sigma \varphi = f, \quad (15)$$

where φ is the *concentration of pollutants*, (u, v, w) are the components of the wind velocity, $w_g = \text{const} > 0$ the falling velocity of the pollutants by gravity, f the power of the source, $\sigma = \text{const} \geq 0$ the transformation coefficient of pollutants and μ, ν are the horizontal and vertical diffusion coefficients.

In many practical situations, e.g. the substance propagation in rivers, the stationary problem of air pollution generated by a point source (modeled by a Dirac delta function) can be reduced to the *one–dimensional advection–diffusion equation*

$$\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} - \mu \frac{\partial^2 \varphi}{\partial x^2} + \sigma \varphi = f, \quad x > 0, \quad t > 0. \quad (16)$$

This is an inhomogeneous version of the considered equation (1).

Besides, the two–dimensional or three–dimensional equations by the *splitting method* [12] or *local one–dimensional* (LOD) method [13,14] are also reduced to the one–dimensional equation (16). Therefore, the equation (16) has attracted great attention from many researchers. A suitable numerical method for solving (16) must guarantee the positivity of the solution, since *negative values* would loose the physical meaning of a concentration. Dang and Ehrhardt [1] proposed a so-called monotone difference scheme to ensure the positivity of the solution.

We will turn to the main part of this work, the subequation method [4].

4 The Subequation Method

In this section, we will explain in detail the subequation method to obtain a NSFD for the convection-diffusion PDE. To start, let us consider the pure heat equation for the unknown $u = u(x, \tau)$

$$u_\tau = a u_{xx}, \quad x \in \mathbb{R}, \tau > 0. \quad (17)$$

Then, the standard (explicit) finite difference discretization reads

$$\frac{u_j^{n+1} - u_j^n}{\Delta\tau} = a \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2}, \quad j \in \mathbb{Z}, n \in \mathbb{N}_0, \quad (18)$$

i.e.

$$u_j^{n+1} = a\mu(u_{j+1}^n + u_{j-1}^n) + (1 - 2a\mu)u_j^n, \quad (19)$$

with the *parabolic mesh ratio* $\mu = \Delta\tau/(\Delta x)^2$ and the pointwise approximation $u_j^n \approx u(x_j, t_n)$, where $x_j = j\Delta x$, $t_n = n\Delta t$, $j \in \mathbb{Z}$, $n \in \mathbb{N}_0$.

Now *positivity* requires

$$1 - 2a\mu \geq 0. \quad (20)$$

Here, positivity means that solutions of this finite difference scheme obey a *discrete maximum principle*

$$\max_j |u_j^{n+1}| \leq \max_j |u_j^n|, \quad n \in \mathbb{N}_0. \quad (21)$$

A way to ensure this condition (20) is to use the ansatz

$$1 - 2a\mu = \gamma a\mu, \quad \gamma \geq 0, \quad (22)$$

where γ is a parameter whose value we may select. From (22), it follows that

$$\Delta\tau = \frac{(\Delta x)^2}{(2 + \gamma)a}. \quad (23)$$

In practice, we have found that the choice $\gamma = 2$ in (22) gives good stability and smoothness behavior for the solutions.

4.1 An illustrative Example

We want to outline the method of subequations for NSFD schemes using as an illustrative example the equation

$$u_\tau + u_x = u(1 - u), \quad x \in \mathbb{R}, \tau > 0. \quad (24)$$

A *subequation* of (24) is an ordinary differential equation (ODE) or partial differential equation (PDE) obtained by dropping one or more terms appearing in the full equation (24). Thus, we have from (24) the following three subequations

$$u_\tau = u(1 - u), \quad \text{an ODE} \quad (25a)$$

$$u_x = u(1 - u), \quad \text{an ODE} \quad (25b)$$

$$u_\tau + u_x = 0, \quad \text{a PDE} \quad (25c)$$

All three subequations have known exact schemes, cf. [4,5]. They are respectively

$$\frac{u^{n+1} - u^n}{\Phi_1(\Delta\tau)} = u^n - u^n u^{n+1}, \quad \Phi_1(\Delta\tau) = e^{\Delta\tau} - 1, \quad (26a)$$

$$\frac{u_{j+1} - u_j}{\Phi_2(\Delta x)} = u_j - u_j u_{j+1}, \quad \Phi_2(\Delta x) = e^{\Delta x} - 1, \quad (26b)$$

$$\frac{u_j^{n+1} - u_j^n}{\Psi(\Delta\tau)} + \frac{u_j^n - u_{j-1}^n}{\Psi(\Delta x)} = 0, \quad \Delta\tau = \Delta x. \quad (26c)$$

Note that for $u_\tau + u_x = 0$, we have a relationship between the step sizes, i.e. $\Delta\tau = \Delta x$. Further, any function $\Psi(z)$ can be used as a *denominator function*, as long as

$$\Psi(z) = z + O(z^2). \quad (27)$$

The issue is to combine the equations (26) into a scheme for (24). For the above three subequations (26), the only way to do this results in the scheme

$$\frac{u_j^{n+1} - u_j^n}{\Phi(h)} + \frac{u_j^n - u_{j-1}^n}{\Phi(h)} = u_{j-1}^n - u_{j-1}^n u_j^{n+1}, \quad (28)$$

where

$$\Phi(h) = e^h - 1, \quad h = \Delta\tau = \Delta x. \quad (29)$$

In fact, (28) can be shown to be the *exact NSFD scheme* [5] for (24).

We briefly check this result. First we consider the space independent equation (25a) and drop the j -dependence in (28) to obtain

$$\frac{u^{n+1} - u^n}{\Phi(\Delta\tau)} = u^n - u^n u^{n+1}, \quad \Phi(\Delta\tau) = e^{\Delta\tau} - 1. \quad (30)$$

For the time-independent equation (25b) we drop the n -dependence in (28) to get after an index shift $j \rightarrow j + 1$

$$\frac{u_{j+1} - u_j}{\Phi(\Delta x)} = u_j - u_j u_{j+1}, \quad \Phi(\Delta x) = e^{\Delta x} - 1. \quad (31)$$

Finally, dropping the terms on the right hand side of (28) gives

$$\frac{u_j^{n+1} - u_j^n}{\Phi(h)} + \frac{u_j^n - u_{j-1}^n}{\Phi(h)} = 0, \quad \Phi(h) = e^h - 1, \quad (32)$$

with $h = \Delta\tau = \Delta x$.

4.2 The Nonstandard Difference Scheme for the Linear Convection-Diffusion-Reaction Equation

We consider a convection-diffusion PDE for the unknown $u = u(x, \tau)$

$$u_\tau + b u_x = a u_{xx} - c u, \quad x \in \mathbb{R}, \tau \geq 0 \quad (33)$$

In general, the diffusion coefficient $a > 0$ and the reaction rate $c > 0$, but the convection speed b may have either sign. In this work we assume for simplicity $b > 0$, but the other case where $b < 0$ can be treated analogously.

The NSFD methodology requires the use of the so-called *upwinding* for the advection term. It is not really relevant that this also is needed in some of the simple standard finite difference schemes. Our NSFD scheme has no choice but to use this structure since we wish to have the positivity condition hold.

In the preceding subsection 4.1 we used three subequations to construct a NSFD scheme for the original PDE (24). For the PDE (33) there are six subequations, but, in general we cannot use all of them. The NSFD scheme for the general convection-diffusion equation (33) proposed here used the following four subequations

$$u_\tau = -c u, \quad \text{an ODE} \quad (34a)$$

$$0 = a u_{xx} - c u, \quad \text{an ODE} \quad (34b)$$

$$u_\tau = b u_x, \quad \text{a PDE} \quad (34c)$$

$$0 = b u_x - c u, \quad \text{a ODE} \quad (34d)$$

All four subequations have known exact schemes, cf. [4].

4.3 The Case without Reaction

Let us first consider the special case without reaction rate, i.e. we consider (33) with $c = 0$:

$$u_\tau + b u_x = a u_{xx}, \quad x \in \mathbb{R}, \tau \geq 0. \quad (35)$$

The explicit (upwind) scheme for (33) is:

$$\frac{u_j^{n+1} - u_j^n}{\Delta\tau} + b \frac{u_j^n - u_{j-1}^n}{\Delta x} = a \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}, \quad j \in \mathbb{Z}. \quad (36)$$

$n \in \mathbb{N}_0$. Now define the parabolic and hyperbolic mesh ratios as

$$\mu = \frac{\Delta\tau}{\Delta x^2}, \quad \lambda = \frac{\Delta\tau}{\Delta x}, \quad \text{with } \Delta\tau = \Delta\tau(a, b, \gamma_{1,2}), \quad (37)$$

then (36) becomes

$$u_j^{n+1} = a\mu u_{j+1}^n + (b\lambda + a\mu)u_{j-1}^n + (1 - b\lambda - 2a\mu)u_j^n. \quad (38)$$

Now, positivity requires $1 - b\lambda - 2a\mu \geq 0$. To proceed, we introduce two parameters $\gamma_1 \geq 0$, $\gamma_2 \geq 0$. The following two cases are allowed

Case A

$$1 - b\lambda - 2a\mu = \gamma_1 a\mu \quad (39)$$

Then we have the scheme

$$u_j^{n+1} = a\mu u_{j+1}^n + (b\lambda + a\mu)u_{j-1}^n + \gamma_1 a\mu u_j^n. \quad (40)$$

with

$$\Delta\tau = \frac{\Delta x^2}{(2 + \gamma_1)a + b\Delta x} \quad (41)$$

$$\lambda = \frac{\Delta x}{(2 + \gamma_1)a + b\Delta x}, \quad \mu = \frac{1}{(2 + \gamma_1)a + b\Delta x}. \quad (42)$$

Case B

$$1 - b\lambda - 2a\mu = \gamma_2 b\lambda \quad (43)$$

Then we have the scheme

$$u_j^{n+1} = a\mu u_{j+1}^n + (b\lambda + a\mu)u_{j-1}^n + \gamma_2 b\lambda u_j^n. \quad (44)$$

with

$$\Delta\tau = \frac{\Delta x^2}{2a + (1 + \gamma_2)b\Delta x} \quad (45)$$

$$\lambda = \frac{\Delta x}{2a + (1 + \gamma_2)b\Delta x}, \quad \mu = \frac{1}{2a + (1 + \gamma_2)b\Delta x}. \quad (46)$$

For both cases A and B one can show that

$$u_j^n \geq u_j^{n+1} \geq 0, \quad (47)$$

i.e. bounded positive input gives bounded positive numerical solutions.

4.4 Subequation Technique for the full PDE

We have the following six *subequations* of the full PDE (33):

$$u_\tau = -c u, \quad \text{an ODE} \quad (48a)$$

$$0 = a u_{xx} - c u, \quad \text{an ODE} \quad (48b)$$

$$u_\tau + b u_x = 0, \quad \text{a PDE} \quad (48c)$$

$$b u_x = -c u, \quad \text{an ODE} \quad (48d)$$

$$b u_x = a u_{xx}, \quad \text{an ODE} \quad (48e)$$

$$u_\tau = a u_{xx}, \quad \text{a PDE} \quad (48f)$$

The first five of (48) have exact schemes, cf. [4]. We will now give a novel scheme that incorporates the exact schemes of the first four equations. The resulting NSFD scheme for (33) is:

$$\frac{u_j^{n+1} - u_j^n}{\frac{1-e^{-c\Delta\tau}}{c}} + b \left\{ \frac{u_j^n - u_{j-1}^n}{\frac{e^{\frac{c\Delta x}{b}} - 1}{\frac{c}{b}}} \right\} = a \left\{ \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\frac{4 \sinh^2[\sqrt{\frac{c}{a}} \frac{\Delta x}{2}]}{\frac{c}{a}}} \right\} - c u_j^n, \quad (49)$$

with $j \in \mathbb{Z}$, $n \in \mathbb{N}_0$.

In the sequel we will give some more insight to (49) and show that the three *denominator functions* are given by the expressions

$$\Phi_1(\Delta\tau, c) = \frac{1 - e^{-c\Delta\tau}}{c}, \quad (50a)$$

$$\Phi_2(\Delta x, a, c) = \frac{4a}{c} \sinh^2 \left[\sqrt{\frac{c}{a}} \frac{\Delta x}{2} \right], \quad (50b)$$

$$\Phi_3(\Delta x, b, c) = \frac{e^{\frac{c\Delta x}{b}} - 1}{\frac{c}{b}}, \quad (50c)$$

as written above. Consequently, the NSFD scheme (49) takes the form

$$\frac{u_j^{n+1} - u_j^n}{\Phi_1(\Delta\tau, c)} + b \frac{u_j^n - u_{j-1}^n}{\Phi_3(\Delta x, b, c)} = a \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Phi_2(\Delta x, a, c)} - c u_j^n. \quad (51)$$

Further, let

$$\begin{aligned} \mu(\Delta\tau, \Delta x, a, c) &\equiv \frac{\Phi_1(\Delta\tau, c)}{\Phi_2(\Delta x, a, c)}, \\ \lambda(\Delta\tau, \Delta x, b, c) &\equiv \frac{\Phi_1(\Delta\tau, c)}{\Phi_3(\Delta x, b, c)}. \end{aligned} \quad (52)$$

This allows us to rewrite the *explicit scheme* (51) as

$$u_j^{n+1} = a\mu u_{j+1}^n + (b\lambda + a\mu)u_{j-1}^n + (1 - b\lambda - 2a\mu - c\Phi_1)u_j^n. \quad (53)$$

Now, for *positivity* we require that in (53) the coefficient

$$1 - b\lambda - 2a\mu - c\Phi_1 = e^{-c\Delta\tau} - 2a\mu - b\lambda \geq 0 \quad (54)$$

must be positive. To ensure this, we set this coefficient equal to $\gamma(2a\mu + b\lambda)$ and immediately obtain for the parameter γ

$$\gamma = \frac{e^{-c\Delta\tau}}{2a\mu + b\lambda} - 1. \quad (55)$$

Hence, finally the NSFD scheme (53) reads

$$u_j^{n+1} = a\mu u_{j+1}^n + \gamma[2a\mu + b\lambda]u_j^n + [b\lambda + a\mu]u_{j-1}^n, \quad (56)$$

with

$$\Delta\tau = \frac{1}{c} \ln \left\{ \frac{1}{1 + \gamma} \frac{1}{2a\mu + b\lambda} \right\}, \quad (57a)$$

$$\text{with } 2a\mu = \frac{1 - e^{-c\Delta\tau}}{2 \sinh^2 \left[\sqrt{\frac{c}{a}} \frac{\Delta x}{2} \right]}, \quad (57b)$$

$$b\lambda = \frac{1 - e^{-c\Delta\tau}}{e^{\frac{c\Delta x}{b}} - 1}. \quad (57c)$$

Since the non-constant mesh ratios μ and λ depend on $\Delta\tau$ and Δx , we have a functional relationship between them. An elementary calculation gives

$$\Delta\tau = \frac{1}{c} \ln \left\{ 1 + \frac{1}{1 + \gamma} \frac{2 \left(e^{\frac{c\Delta x}{b}} - 1 \right) \sinh^2 \left[\sqrt{\frac{c}{a}} \frac{\Delta x}{2} \right]}{e^{\frac{c\Delta x}{b}} - 1 + 2 \sinh^2 \left[\sqrt{\frac{c}{a}} \frac{\Delta x}{2} \right]} \right\}, \quad (58)$$

which is a nonlinear equation to determine the time step since γ depends on $\Delta\tau$, cf. (55).

We conclude this section by summarizing the resulting algorithm which should be carried out to obtain the required numerical solution:

Algorithm 1

- (1) *Input parameters: a, b, c .*
- (2) *Select a value for $\gamma \geq 0$.*
- (3) *Choose the spatial step size Δx .*
- (4) *Calculate the time step $\Delta\tau$ from (58).*
- (5) *Calculate the ratios μ and λ from (52) using (50).*
- (6) *Using the initial and boundary-value data, apply the explicit finite difference scheme (56) to determine a numerical solution.*
If $c = 0$, then use the scheme from Section 4.3 instead.

Remark 1 Another way of deriving a (different) NSFD scheme for the full PDE (33) is based on the classical separation of variables approach that leads to the solution of two ODEs having well-known NSFD schemes, cf. [4,5]. However, here we prefer the subequation methods, since it involves directly PDEs.

5 The Modified Equation Analysis

In this section we study the effects of the discretization on the dispersion and dissipation by the *modified equation technique* [15,16]. The idea is to describe the qualitative behaviour of the solutions to the finite difference approximation, i.e. mainly the dissipation and dispersion errors, by an analytic PDE with mesh dependent coefficients for which the finite difference method (FDM) has a higher order of consistency.

5.1 The Effect of the Spatial Discretization

5.1.1 The Centered-in-Space Scheme

We start with considering a standard spatial discretization of (33) using a central difference quotient for the convection term:

$$\begin{aligned} \partial_\tau u_j(\tau) + b \frac{u_{j+1}(\tau) - u_{j-1}(\tau)}{2\Delta x} \\ = a \frac{u_{j+1}(\tau) - 2u_j(\tau) + u_{j-1}(\tau)}{\Delta x^2} - c u_j(\tau), \end{aligned} \quad (59)$$

$j \in \mathbb{Z}$, $\tau \geq 0$, where $u_j(\tau) \approx u(j\Delta x, \tau)$. Next, assume the existence of a smooth solution $u(x, \tau)$ to the PDE with the values $u(x_j, \tau) = u_j(\tau)$ at the spatial grid points x_j and expand the solution $u_j(\tau)$ in Taylor series around $x_j = j\Delta x$ to obtain the modified PDE

$$u_\tau + b u_x + b \frac{\Delta x^2}{6} u_{xxx} = a u_{xx} + a \frac{\Delta x^2}{12} u_{xxxx} - c u + O(\Delta x^4), \quad (60)$$

$x \in \mathbb{R}$, $\tau \geq 0$. We insert an appropriate Fourier-type solution of the form:

$$u(x, \tau) = \exp\{-(A + c)\tau\} \exp\{ik(x - B\tau)\}, \quad (61)$$

that consist of an exponential modelling the dissipation (+ reaction) effects and a second exponential that represents the convection, and solve for A and B :

$$A = a \left[1 - \frac{\Delta x^2}{12} k^2 \right] k^2, \quad B = b \left[1 - \frac{\Delta x^2}{6} k^2 \right] \quad (62)$$

and one can easily study in (62) how the deviations in dissipation and convection speed depending on the spatial grid size Δx and the wave number k . In this case of centered differences the discretization leads to a reduction of the effect of diffusion and convection.

5.1.2 The Upwind Scheme

Analogously, one gets for the upwind discretization

$$\begin{aligned} u_\tau + b u_x + b \frac{\Delta x^2}{6} u_{xxx} \\ = \left[a + b \frac{\Delta x}{2} \right] u_{xx} + \left[a \frac{\Delta x^2}{12} + b \frac{\Delta x^3}{24} \right] u_{xxxx} - c u + O(\Delta x^4), \end{aligned} \quad (63)$$

having a Fourier-type solution (61) with

$$A = \left[a + b \frac{\Delta x}{2} \right] \left[1 - \frac{\Delta x^2}{12} k^2 \right] k^2, \quad B = b \left[1 - \frac{\Delta x^2}{6} k^2 \right], \quad (64)$$

i.e. the upwind discretization yields some additional artificial dissipation of magnitude $b\Delta x/2$.

5.1.3 The NSFD Scheme

Next, we consider the time-continuous version of the NSFD scheme (51) with the two denominator functions Φ_2 , Φ_3 , given in (50)

$$\begin{aligned} \partial_\tau u_j(\tau) + b \frac{u_j(\tau) - u_{j-1}(\tau)}{\Phi_3(\Delta x, b, c)} \\ = a \frac{u_{j+1}(\tau) - 2u_j(\tau) + u_{j-1}(\tau)}{\Phi_2(\Delta x, a, c)} - c u_j(\tau), \end{aligned} \quad (65)$$

with the expansion

$$\Phi_2(\Delta x, a, c) = \Delta x^2 + \frac{c}{a} \frac{\Delta x^4}{12} + O(\Delta x^6).$$

Now, a tedious, but elementary calculation yields

$$\begin{aligned} u_\tau + b \left[1 - \frac{c}{b} \frac{\Delta x}{2} + \left(\frac{c}{b} \right)^2 \frac{\Delta x^2}{12} + \left(\frac{c}{b} \right)^2 \frac{\Delta x^3}{24} \right] u_x \\ + b \frac{\Delta x^2}{6} \left[1 - \frac{c}{b} \frac{\Delta x}{2} \right] u_{xxx} \\ = \left[a \left(1 - \frac{c}{a} \frac{\Delta x^2}{12} \right) + b \frac{\Delta x}{2} \left(1 - \frac{c}{b} \frac{\Delta x}{2} + \left(\frac{c}{b} \right)^2 \frac{\Delta x^2}{12} \right) \right] u_{xx} \\ + \left[a \frac{\Delta x^2}{12} + b \frac{\Delta x^3}{24} \right] u_{xxxx} - c u + O(\Delta x^4), \end{aligned} \quad (66)$$

cf. (63), having a Fourier-type solution (61) with

$$\begin{aligned}
A &= \left[a + b \frac{\Delta x}{2} \right] \left[1 - \frac{\Delta x^2}{12} k^2 \right] k^2 - c \frac{\Delta x^2}{3} \left[1 - \frac{c}{b} \frac{\Delta x}{8} \right] k^2, \\
B &= b \left[1 - \frac{c}{b} \frac{\Delta x}{2} + \left(\frac{c}{b} \right)^2 \frac{\Delta x^2}{12} + \left(\frac{c}{b} \right)^2 \frac{\Delta x^3}{24} \right] \\
&\quad - b \frac{\Delta x^2}{6} \left[1 - \frac{c}{b} \frac{\Delta x}{2} \right].
\end{aligned} \tag{67}$$

Compared to (64) we observe that both the dissipation and convection coefficients in the Fourier solution are reduced by correction terms that depend on the reaction rate c , especially the ratio of reaction to convection c/b .

The effect of the time discretization can be analyzed analogously.

Remark 2 (Financial Interpretation) *If the PDE (33) is considered in a financial context, then the above analysis shows that the centered difference discretization leads to a lower volatility and a lower drift. Both perturbations are proportional to the square of the spatial frequency (wave number) k , i.e. non-smooth pay-offs (3) stimulates these distortions, since high spatial frequencies are induced.*

5.2 Analysis of the Fully Discrete Scheme

5.2.1 The Upwind Scheme

To begin, we start with explaining the method using the upwind scheme, cf. (36). We use Taylor series around the point (x_j, t_n) and insert it into the difference scheme to obtain

$$\begin{aligned}
&\left(\frac{\partial u}{\partial \tau} \right)_j^n + \frac{\Delta \tau}{2} \left(\frac{\partial^2 u}{\partial \tau^2} \right)_j^n + \frac{\Delta \tau^2}{6} \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n + \mathcal{O}(\Delta \tau^3) \\
&\quad + b \left(\frac{\partial u}{\partial x} \right)_j^n - b \frac{\Delta x}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n + b \frac{\Delta x^2}{6} \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n \\
&= a \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n + a \frac{\Delta x^2}{12} \left(\frac{\partial^4 u}{\partial x^4} \right)_j^n - c (u)_j^n + \mathcal{O}(\Delta x^3).
\end{aligned} \tag{68}$$

This modified equation consists of the original PDE plus the terms stemming from the truncation error of the scheme.

The next (tedious) step is to replace all time derivatives with order higher than one in (68) by spatial derivatives. To do so, we differentiate (68) with

respect to τ

$$\begin{aligned}
& \left(\frac{\partial^2 u}{\partial \tau^2} \right)_j^n + \frac{\Delta \tau}{2} \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n + O(\Delta \tau^2) \\
& + b \left(\frac{\partial^2 u}{\partial x \partial \tau} \right)_j^n - b \frac{\Delta x}{2} \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n + b \frac{\Delta x^2}{6} \left(\frac{\partial^4 u}{\partial x^3 \partial \tau} \right)_j^n \\
& = a \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n + a \frac{\Delta x^2}{12} \left(\frac{\partial^5 u}{\partial x^4 \partial \tau} \right)_j^n - c \left(\frac{\partial u}{\partial \tau} \right)_j^n + O(\Delta x^3),
\end{aligned} \tag{69}$$

and differentiate (68) with respect to x and multiply by b

$$\begin{aligned}
& b \left(\frac{\partial u^2}{\partial x \partial \tau} \right)_j^n + b \frac{\Delta \tau}{2} \left(\frac{\partial^3 u}{\partial x \partial \tau^2} \right)_j^n + O(\Delta \tau^2) \\
& + b^2 \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n - b^2 \frac{\Delta x}{2} \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n + b^2 \frac{\Delta x^2}{6} \left(\frac{\partial^4 u}{\partial x^4} \right)_j^n \\
& = ab \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n + ab \frac{\Delta x^2}{12} \left(\frac{\partial^5 u}{\partial x^5} \right)_j^n - bc \left(\frac{\partial u}{\partial x} \right)_j^n + O(\Delta x^3).
\end{aligned} \tag{70}$$

Now subtracting (70) from (69) and replacing the first time derivative by (68) gives

$$\begin{aligned}
& \left[1 - c \frac{\Delta \tau}{2} \right] \left(\frac{\partial^2 u}{\partial \tau^2} \right)_j^n = 2bc \left(\frac{\partial u}{\partial x} \right)_j^n + (b^2 - ac) \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n \\
& - ab \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n + c^2 (u)_j^n + a \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n \\
& + \frac{\Delta \tau}{2} \left[b \left(\frac{\partial^3 u}{\partial x \partial \tau^2} \right)_j^n - \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n \right] + O(\Delta \tau^2) \\
& + b \frac{\Delta x}{2} \left[\left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n - b \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n - c \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n \right] + O(\Delta x^2).
\end{aligned} \tag{71}$$

The next step is to replace any term in (71) involving a time derivative, i.e.

$$\left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n, \quad \left(\frac{\partial^3 u}{\partial x \partial \tau^2} \right)_j^n, \quad \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n.$$

For example, the first term can be expressed by differentiating (70) with respect to x :

$$\begin{aligned}
& \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n = a \left(\frac{\partial^4 u}{\partial x^4} \right)_j^n - b \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n - c \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n \\
& - \frac{\Delta \tau}{2} \left(\frac{\partial^4 u}{\partial x^2 \partial \tau^2} \right)_j^n + b \frac{\Delta x}{2} \left(\frac{\partial^4 u}{\partial x^4} \right)_j^n + O(\Delta \tau^2) + O(\Delta x^2),
\end{aligned} \tag{72}$$

and inserting it into (71) yields up to first order the result

$$\begin{aligned} \left(\frac{\partial^2 u}{\partial \tau^2}\right)_j^n &= a^2 \left(\frac{\partial^4 u}{\partial x^4}\right)_j^n + 2bc \left(\frac{\partial u}{\partial x}\right)_j^n + (b^2 - 2ac) \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n \\ &\quad - 2ab \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n + c^2 (u)_j^n + O(\Delta \tau) + O(\Delta x). \end{aligned} \quad (73)$$

A final substitution into (68) gives the *modified equation*

$$\begin{aligned} \left(\frac{\partial u}{\partial \tau}\right)_j^n &= \left[a + (2ac - b^2) \frac{\Delta \tau}{2} + b \frac{\Delta x}{2} \right] \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n \\ &\quad - b \left[1 + c \Delta \tau \right] \left(\frac{\partial u}{\partial x}\right)_j^n - c \left[1 + c \frac{\Delta \tau}{2} \right] (u)_j^n + O(\Delta x^2) \\ &\quad + ab \Delta \tau \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n - a^2 \frac{\Delta \tau}{2} \left(\frac{\partial^4 u}{\partial x^4}\right)_j^n + O(\Delta \tau^2), \end{aligned} \quad (74)$$

that allows us to study how numerical diffusion and numerical dispersion is introduced by the upwind scheme. To investigate higher order effects, higher order time derivatives in (71) must be eliminated.

5.2.2 The NSFD Scheme

Secondly, if we consider the NSFD scheme (51) we obtain instead of (68) the equation

$$\begin{aligned} &\left[1 + c \frac{\Delta \tau}{2} + c^2 \frac{\Delta \tau^2}{12} \right] \left(\frac{\partial u}{\partial \tau}\right)_j^n \\ &+ \frac{\Delta \tau}{2} \left[1 + c \frac{\Delta \tau}{2} \right] \left(\frac{\partial^2 u}{\partial \tau^2}\right)_j^n + \frac{\Delta \tau^2}{6} \left(\frac{\partial^3 u}{\partial \tau^3}\right)_j^n + O(\Delta \tau^3) \\ &+ b \left[1 - \frac{c}{b} \frac{\Delta x}{2} + \left(\frac{c}{b}\right)^2 \frac{\Delta x^2}{12} + \left(\frac{c}{b}\right)^2 \frac{\Delta x^3}{24} \right] \left(\frac{\partial u}{\partial x}\right)_j^n \\ &\quad + b \frac{\Delta x^2}{6} \left[1 - \frac{c}{b} \frac{\Delta x}{2} \right] \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n \\ &= \left[a \left(1 - \frac{c}{a} \frac{\Delta x^2}{12} \right) + b \frac{\Delta x}{2} \left(1 - \frac{c}{b} \frac{\Delta x}{2} + \left(\frac{c}{b}\right)^2 \frac{\Delta x^2}{12} \right) \right] \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n \\ &\quad + \left[a \frac{\Delta x^2}{12} + b \frac{\Delta x^3}{24} \right] \left(\frac{\partial^4 u}{\partial x^4}\right)_j^n - c (u)_j^n + O(\Delta x^4), \end{aligned} \quad (75)$$

where the time derivatives with order higher than one can be eliminated following exactly the same strategy as before, i.e. we replace all time derivatives with order higher than one in (75) by spatial derivatives. First, we differentiate

(75) with respect to the time τ

$$\begin{aligned}
& \left[1 + c \frac{\Delta\tau}{2} \right] \left(\frac{\partial^2 u}{\partial \tau^2} \right)_j^n + \frac{\Delta\tau}{2} \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n + \text{O}(\Delta\tau^2) \\
& \quad + b \left[1 - \frac{c \Delta x}{b} \frac{\Delta x}{2} \right] \left(\frac{\partial^2 u}{\partial x \partial \tau} \right)_j^n \\
& = \left[a + b \frac{\Delta x}{2} \right] \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n - c \left(\frac{\partial u}{\partial \tau} \right)_j^n + \text{O}(\Delta x^2).
\end{aligned} \tag{76}$$

To eliminate the mixed derivative we and differentiate (75) with respect to x and multiply by the *perturbed convection speed*

$$\tilde{b} = b \frac{1 - \frac{c \Delta x}{b} \frac{\Delta x}{2}}{1 + c \frac{\Delta\tau}{2}},$$

yielding

$$\begin{aligned}
& b \left[1 - \frac{c \Delta x}{b} \frac{\Delta x}{2} \right] \left(\frac{\partial^2 u}{\partial x \partial \tau} \right)_j^n + \tilde{b} \frac{\Delta\tau}{2} \left(\frac{\partial^3 u}{\partial x \partial \tau^2} \right)_j^n + \text{O}(\Delta\tau^2) \\
& \quad + \tilde{b} b \left[1 - \frac{c \Delta x}{b} \frac{\Delta x}{2} \right] \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n \\
& = \tilde{b} \left[a + b \frac{\Delta x}{2} \right] \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n - \tilde{b} c \left(\frac{\partial u}{\partial x} \right)_j^n + \text{O}(\Delta x^2).
\end{aligned} \tag{77}$$

Next, subtracting (77) from (76) gives

$$\begin{aligned}
& \left[1 + c \frac{\Delta\tau}{2} \right] \left(\frac{\partial^2 u}{\partial \tau^2} \right)_j^n = - \frac{\Delta\tau}{2} \left(\frac{\partial^3 u}{\partial \tau^3} \right)_j^n + \tilde{b} \frac{\Delta\tau}{2} \left(\frac{\partial^3 u}{\partial x \partial \tau^2} \right)_j^n + \text{O}(\Delta\tau^2) \\
& \quad + \tilde{b} b \left[1 - \frac{c \Delta x}{b} \frac{\Delta x}{2} \right] \left(\frac{\partial^2 u}{\partial x^2} \right)_j^n + \left[a + b \frac{\Delta x}{2} \right] \left(\frac{\partial^3 u}{\partial x^2 \partial \tau} \right)_j^n \\
& \quad - c \left(\frac{\partial u}{\partial \tau} \right)_j^n - \tilde{b} \left[a + b \frac{\Delta x}{2} \right] \left(\frac{\partial^3 u}{\partial x^3} \right)_j^n + \tilde{b} c \left(\frac{\partial u}{\partial x} \right)_j^n + \text{O}(\Delta x^2),
\end{aligned}$$

multiplying by $1 + c\Delta\tau/2$ and replacing the first time derivative by (75) gives

$$\begin{aligned}
\left[1 + c\frac{\Delta\tau}{2}\right]^2 \left(\frac{\partial^2 u}{\partial\tau^2}\right)_j^n &= \left[\left(b - c\frac{\Delta x}{2}\right)^2 - c\left(a + b\frac{\Delta x}{2}\right)\right] \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n \\
&\quad - \frac{\Delta\tau}{2} \left[1 + c\frac{\Delta\tau}{2}\right] \left(\frac{\partial^3 u}{\partial\tau^3}\right)_j^n + \frac{\Delta\tau}{2} \left(b - c\frac{\Delta x}{2}\right) \left(\frac{\partial^3 u}{\partial x \partial\tau^2}\right)_j^n \\
&\quad + \left[a + b\frac{\Delta x}{2}\right] \left[1 + c\frac{\Delta\tau}{2}\right] \left(\frac{\partial^3 u}{\partial x^2 \partial\tau}\right)_j^n + O(\Delta\tau^2) \\
&\quad - \left[a + b\frac{\Delta x}{2}\right] \left(b - c\frac{\Delta x}{2}\right) \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n + c^2(u)_j^n \\
&\quad + 2c \left[b - c\frac{\Delta x}{2}\right] \left(\frac{\partial u}{\partial x}\right)_j^n + O(\Delta x^2).
\end{aligned} \tag{78}$$

Now we replace the mixed term (78)

$$\left[1 + c\frac{\Delta\tau}{2}\right] \left(\frac{\partial^3 u}{\partial x^2 \partial\tau}\right)_j^n$$

by differentiating (75) two times with respect to x . This procedure yields up to first order

$$\begin{aligned}
\left[1 + c\frac{\Delta\tau}{2}\right]^2 \left(\frac{\partial^2 u}{\partial\tau^2}\right)_j^n &= \left[\left(b - c\frac{\Delta x}{2}\right)^2 - c\left(a + b\frac{\Delta x}{2}\right)\right] \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n \\
&\quad - \frac{\Delta\tau}{2} \left[1 + c\frac{\Delta\tau}{2}\right] \left(\frac{\partial^3 u}{\partial\tau^3}\right)_j^n + \frac{\Delta\tau}{2} \left(b - c\frac{\Delta x}{2}\right) \left(\frac{\partial^3 u}{\partial x \partial\tau^2}\right)_j^n \\
&\quad + \left[a + b\frac{\Delta x}{2}\right]^2 \left(\frac{\partial^4 u}{\partial x^4}\right)_j^n + \frac{\Delta\tau}{2} \left[a + b\frac{\Delta x}{2}\right] \left(\frac{\partial^4 u}{\partial x^2 \partial\tau^2}\right)_j^n \\
&\quad - 2 \left[a + b\frac{\Delta x}{2}\right] \left(b - c\frac{\Delta x}{2}\right) \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n + c^2(u)_j^n + O(\Delta\tau^2) \\
&\quad + 2c \left[b - c\frac{\Delta x}{2}\right] \left(\frac{\partial u}{\partial x}\right)_j^n + O(\Delta x^2).
\end{aligned} \tag{79}$$

Finally we substitute (79) in (75), multiplied by $1 + c\Delta\tau/2$, and obtain the *modified equation for the NSFD scheme*

$$\begin{aligned}
\left(\frac{\partial u}{\partial\tau}\right)_j^n &= \left[a + \frac{b\Delta x - \Delta\tau}{2(1 + c\Delta t)}\right] \left(\frac{\partial^2 u}{\partial x^2}\right)_j^n - b \left[1 - \frac{c}{2b} \frac{\Delta x}{1 + c\Delta t}\right] \left(\frac{\partial u}{\partial x}\right)_j^n \\
&\quad - c(u)_j^n + ab \frac{\Delta\tau}{1 + c\Delta t} \left(\frac{\partial^3 u}{\partial x^3}\right)_j^n - a^2 \frac{\Delta\tau}{2(1 + c\Delta t)} \left(\frac{\partial^4 u}{\partial x^4}\right)_j^n \\
&\quad + O(\Delta\tau^2) + O(\Delta x^2),
\end{aligned} \tag{80}$$

with $\Delta\tau$ implicitly given by the nonlinear equation (58).

Next, one can compare the two modified equations of the upwind scheme (74) and of the NSFD scheme (80) to study the different qualitative behavior by observing the numerical diffusion and dispersion errors. E.g. it can be realized that the NSFD method reproduces better the effect of the reaction rate c .

Remark 3 *Alternatively, following the work of Junk and Yang [17], one can use asymptotic methods, such as (discrete) multiscale expansions to analyse the properties of the finite difference methods, e.g. an upwind discretization is investigated in [17, Section 2.4].*

6 Numerical Results

In this section we compare the results of our new proposed NSFD scheme with the two classical explicit finite difference methods presented earlier. However, for the numerical tests, we consider the case $c = 0$, i.e.

$$u_\tau + b u_x = a u_{xx}, \quad (81)$$

with $a > 0$ and positive convection $b \geq 0$, which was considered in §4.3. For the comparison we use two classical explicit schemes: the *centered-in-space discretization*

$$u_j^{n+1} = u_j^n - \frac{b\lambda}{2}(u_{j+1}^n - u_{j-1}^n) + a\mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \quad (82)$$

i.e.

$$u_j^{n+1} = a\mu[1 + \text{Pe}]u_{j-1}^n + [1 - 2a\mu]u_j^n + a\mu[1 - \text{Pe}]u_{j+1}^n, \quad (83)$$

with the cell Péclet number

$$\text{Pe} := \frac{b\lambda}{2a\mu} = \frac{b\Delta x}{2a}. \quad (84)$$

Secondly, we consider the *upwind differencing* of the convection term

$$u_j^{n+1} = u_j^n - b\lambda(u_j^n - u_{j-1}^n) + a\mu(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \quad (85)$$

i.e.

$$u_j^{n+1} = [a\mu + b\lambda]u_{j-1}^n + [1 - 2a\mu - b\lambda]u_j^n + a\mu u_{j+1}^n, \quad (86)$$

Remark 4 *We note that the upwind scheme (85) can be written as a centered-in-space scheme with added artificial viscosity $a \text{Pe} u_{xx}$:*

$$\frac{u_j^{n+1} - u_j^n}{\Delta\tau} + b \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = a(1 + \text{Pe}) \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}. \quad (87)$$

A von Neumann analysis [10] yields the *stability criterion* for (82)

$$a\mu \leq \frac{1}{2}, \quad \frac{b^2}{a} \Delta t \leq 2 \quad (88)$$

and for the upwind scheme (85)

$$a\mu \leq \left(2 + \left| \frac{b\Delta x}{a} \right| \right)^{-1}, \quad (89)$$

that is valid for both signs of b .

Furthermore, one can easily observe that we need in (83) $Pe \leq 1$ and in (86) $2a\mu + b\lambda \leq 1$ for the *positivity* of the difference scheme. These conditions must be fulfilled such that a discrete maximum principle holds preventing oscillations in the numerical solution.

Example 5 ([18, p. 159]) We choose for the coefficients $a = 0.1$, convection speed $b = 10$, and the spatial step sizes $\Delta x = 1/20$ and $\Delta x = 1/30$ Δt is given by fixing $\mu = 1$, i.e. the cell Péclet number (84) has the value $Pe := 50\Delta x$. As initial data we use the tent function between -0.5 and 0.5 , i.e.

$$u(x, 0) = \begin{cases} 2x + 1, & -0.5 < x < 0 \\ -2x + 1, & 0 \leq x < 0.5, \end{cases}$$

which serves as a model for a non-smooth payoff-function like (3) that stimulates high spatial frequency parts in the solution. For Péclet numbers greater than one it is expected that none of the two standard schemes yield reasonable results, cf. [18].

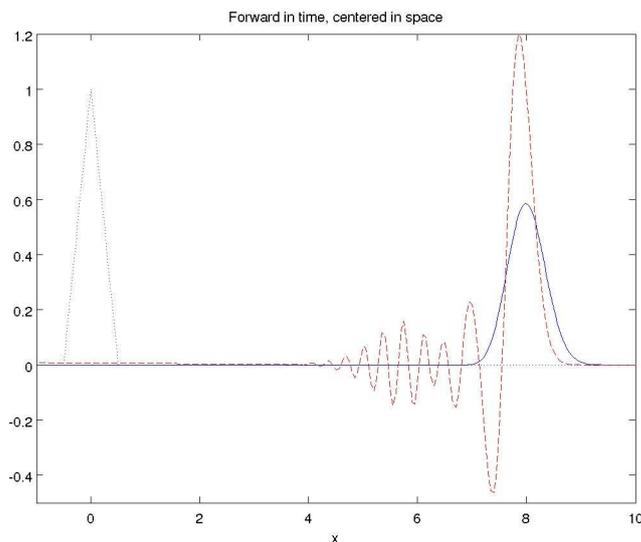


Fig. 1. Forward in time centered in space.

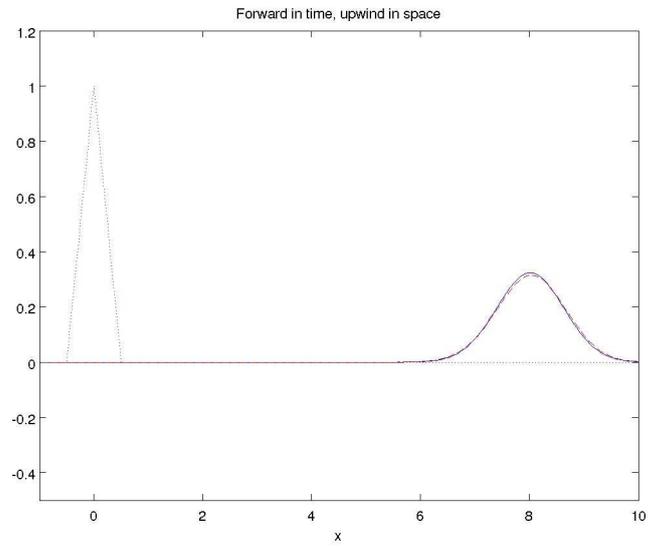


Fig. 2. Forward in time upwind in space.

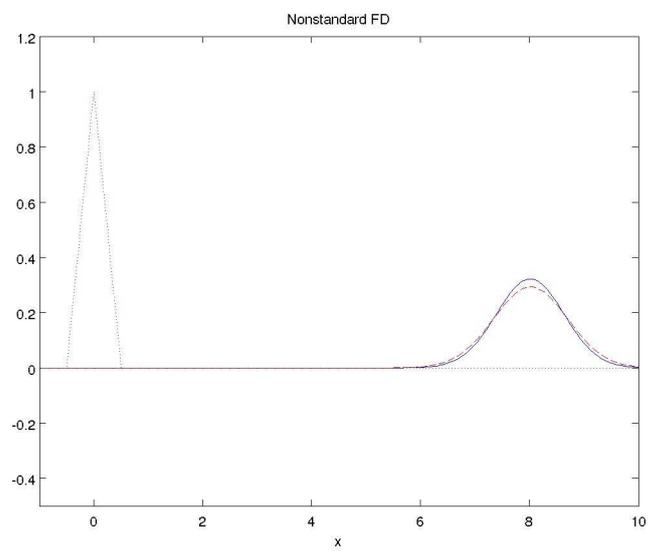


Fig. 3. Nonstandard FD scheme.

In the three figures we plot for each of the three schemes the initial function and the solution at the final time $t = 0.8$ for the spatial step sizes $\Delta x = 1/30$ (blue solid line) and $\Delta x = 1/20$ (red dashed line). The FTCS scheme yields for $\Delta x = 1/20$ an oscillatory solution and for the finer grid the solution is smooth but the values are significantly larger than the exact solution. The upwind and the NSFD scheme show similar results: they eliminate the oscillations, but the solution at $t = 0.8$ is significantly smaller than the exact solution (with a maximum value ≈ 0.44). However, we recall that the NSFD scheme always preserves the positivity of the solution.

7 Conclusion and Outlook

In this paper we have presented a novel nonstandard finite difference (NSFD) method for the solution of a general convection-diffusion PDE that can be used for the linear Black-Scholes equation for pricing standard options.

Although being explicit, this new NSFD scheme has the advantage of preserving the positivity of the solution, which is important in many applications in physics, finance etc.. As a byproduct, this NSFD scheme obeys a discrete maximum principle and thus is stable with respect to the maximum norm. Additionally, the time step restriction of the new NSFD scheme is usually much less restrictive than for standard explicit finite difference schemes.

Our next first goal will be to modify the NSFD scheme to handle more general convection-diffusion equations with non-constant coefficients. Future work will focus on the construction of NSFD schemes for *spatially two dimensional PDEs* and for *nonlinear Black-Scholes equations* [19,20] especially for equations with a nonlinear convective term, cf. [21].

Also, we will derive a NSFD scheme for the original Black-Scholes equation (2) based on an exponentially fitted or finite volume formulation, cf. [22], since often a standard transformation is not possible.

Finally, it is our goal to *bypass any time step restrictions* that are typical for explicit finite difference schemes. One possible way of doing this is to adapt the ideas of Funaro and Pontrelli [23] for constructing implicit schemes for the hyperbolic transport equation to our parabolic problems.

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