DISCRETE ARTIFICIAL BOUNDARY CONDITIONS FOR THE BLACK–SCHOLES EQUATION OF AMERICAN OPTIONS

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Abstract. In this work we derive an exact discrete artificial boundary condition for the Crank–Nicolson scheme for solving the Black–Scholes equation for the valuation of American options.

To ensure stability and to avoid any numerical reflections we derive the artificial boundary condition on a purely discrete level. Since the exact discrete artificial boundary condition includes a convolution with respect to time with a weakly decaying kernel, its numerical evaluation becomes very costly for large–time simulations. As a remedy we construct approximate artificial boundary conditions with a kernel having the form of a finite sum–of–exponentials, which can be evaluated in a very efficient recursion. We prove a simple stability criteria for the approximated artificial boundary conditions. Finally we illustrate the efficiency of the proposed method on several examples and compare it to previously obtained discretized artificial boundary conditions.

Key words. Black–Scholes equation, computational finance, option pricing, finite difference method, artificial boundary condition, stability, free boundary problem, American option

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1. Introduction.

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], [24] and received in 1997 the Nobel Prize in Economics for their discovery [12]. Mathematically it is a final value problem for a second order parabolic equation. A concise derivation of the Black–Scholes equation can be found in [32].

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 E (*'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. We remark that most of the options traded in stock exchanges are of American style. While for European options the Black–Scholes equation results after a standard transformation in a boundary value problem (that can be solved explicitly for cases with constant coefficients and simple payoffs [32]), for American options it results in a free boundary problem for the heat equation.

In general, closed–form solutions do not exist (especially for American options) and the solution has to be computed numerically (cf. the references given in [16]). The standard approach for solving the Black–Scholes equation for American options consists in transforming the original equation to a heat equation posed on a semi–unbounded domain with a free boundary [29], [32]. For a new alternative direct method using the Mellin transformation we refer the reader to [19], [26].

Usually finite differences [30] or finite elements [1] are used to discretize this heat equation and an *artificial boundary condition* (ABC) is introduced in order to confine

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the computational domain appropriately. If the solution on the computational domain coincides with the exact solution on the unbounded domain (restricted to the finite domain), one refers to this boundary condition as a *transparent boundary condition* (TBC). While the numerical treatment of the free boundary has attracted a lot of attention and different strategies were developed (e.g. [8]) less attention was payed to the accurate treatment of the artificial boundary even though the *analytic TBC* for the heat equation is well–known, cf. [15], [27], [34]. In fact, many textbooks propose to use a homogeneous Dirichlet boundary condition at some finite distance [32].

Kangro and Nicolaides considered in [20] a multidimensional Black–Scholes equation for European options and derived pointwise bounds for the error caused by various boundary conditions imposed on the artificial boundary. Windcliff, Forsyth and Vetzal [33] derived necessary stability conditions for a finite difference discretization of the Black–Scholes equation for European options with the common linear asymptotic boundary condition, i.e. assuming that the second derivative of the option value vanishes as the market price becomes large. Recently, Han and Wu [16] proposed a discretization strategy of the analytic TBC to solve the Black–Scholes equation for the American option problem in conjunction with the Crank–Nicolson scheme. The authors also introduced a simple explicit treatment of the free boundary.

However, *ad-hoc discretizations of an analytic TBC* may induce numerical reflections at this artificial boundary and also may destroy the unconditional stability of the Crank–Nicolson finite difference method. To overcome both problems a so–called *discrete TBC* (DTBC) is derived from the fully discretized problem on the unbounded domain. This discrete TBC is completely reflection–free and conserves the stability property of the underlying scheme. Since the discrete TBC includes a convolution with respect to time with a weakly decaying kernel, its numerical evaluation becomes very costly for large–time simulations. As a remedy we construct an *approximate discrete TBC* with a kernel having the form of a finite sum-of-exponentials [3], which can be evaluated by a very efficient recursion formula.

This paper is organized as follows: first we introduce the Black–Scholes equation and recall the standard transformations to a forward–in–time heat equation. In §3 we derive the analytic TBC for the heat equation and for the case of time–dependent parameters. To incorporate the TBC into a finite difference method we review in §4 two approaches to discretize the analytic TBC and construct a DTBC for the Crank–Nicolson discretization. In §6 we discuss the numerical treatment of the free boundary. To reduce the numerical effort we present in §5 an efficient implementation by the sum-of-exponentials approximation. Afterwards we analyze in §7 the stability of the resulting numerical scheme. Finally we illustrate in §8 the accuracy and efficiency of the new method with a numerical example and compare it to the known discretized TBCs of Mayfield [22] and Han and Wu [16].

2. The Black–Scholes equation. In this paper we consider an *American call option*. The treatment of an *American put option* is analogous. The *value of a call option* is denoted by V and depends on the current market price of the underlying asset, S, and the remaining time t until the option expires: $V = V(S,t)$. The *Black–Scholes equation* is a backward–in–time parabolic equation and posed on a time–dependent domain

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + (r - D_0)S\,\frac{\partial V}{\partial S} - rV = 0, \quad 0 < S < S_f(t), \quad 0 \le t < T, \tag{2.1a}$$

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'). We assume that dividends are paid with a continuous yields of constant level $D_0 > 0$. Note that we have to include the payment of dividends. Otherwise, for $D_0 = 0$ early exercise does not make sense and the American call would be equivalent to the European one [24].

In (2.1a) $S_f(t)$ denotes the (a priori unknown) *free boundary* and is also called *'early exercise boundary'* or 'optimal exercise price'. The American call option should be exercised if the value of the asset S is equal or greater than $S_f(t)$ at time t; otherwise the option should be held. Thus the free boundary $S_f(t)$ separates the *holding region* ($S < S_f(t)$) from the *exercise region* ($S \geq S_f(t)$).

The *final condition* ('payoff condition') at the expiry $t = T$ can be written as

$$V(S,T) = (S - E)^+, \qquad 0 \leq S < S_f(T), \tag{2.1b}$$

with the notation $f^+ = \max(f, 0)$. Here $E > 0$ denotes the previously agreed *exercise price* or 'strike', of the contract and $S_f(T) = \max(E, rE/D_0)$.

The 'spatial' or asset–price *boundary conditions* at $S = 0$, and $S = S_f(t)$ are

$$V(0,t) = 0, \qquad 0 \leq t \leq T, \tag{2.1c}$$

$$V(S_f(t),t) = (S_f(t) - E)^+, \quad \frac{\partial V}{\partial S}(S_f(t),t) = 1, \qquad 0 \leq t \leq T, \tag{2.1d}$$

i.e. at $S = 0$ the option is worthless. Note that we need two conditions at the free boundary $S = S_f(t)$. One condition is necessary for the solution of (2.1a) and the other one is needed for determining the position of the free boundary $S_f(t)$ itself. The first condition in (2.1d) ('value matching' condition) is the continuity of the mapping $S \mapsto V(S,t)$ since $V(S,t) = (S - E)^+ = S - E$, in the exercise region $S \geq S_f(t)$. At $S = S_f(t)$ one requires additionally that $V(S,t)$ touches the payoff function tangentially ('high contact condition'), i.e. the function $S \mapsto \partial V(S,t)/\partial S$ should be continuous at $S = S_f(t)$. The conditions (2.1d) are jointly referred as the *'smooth–pasting conditions'*. Note that the later condition can be derived from an arbitrage argument [30], [32].

Since American options can be exercised at any time, we have the *a priori bound*

$$V(S,t) \geq (S - E)^+, \qquad S \geq 0, \quad 0 \leq t \leq T.$$

If $V(S,t) < (S - E)^+$ for one value $S > E$ and $t \leq T$ then the purchase of a call for V and the immediate exercise of this option to buy the underlying asset for E (although its value is S) would lead to an instantaneous risk–free profit of $S - V - E > 0$, in violation to the *no–arbitrage principle*. Of course, this reasoning ignores transaction costs.

2.1. The transformation to the heat equation. In the sequel we shall show how to transform (2.1a) into a pure diffusion equation (cf. [32, § 5.4]). First it is convenient to apply a time reversal and transform (2.1) to a *forward–in–time equation* by the change of variable $t = T - 2\tau/\sigma^2$. 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:

$$\widetilde{V}(S,\tau) = V(S,t) = V\big(S, T - \frac{2\tau}{\sigma^2}\big), \quad \widetilde{S}_f(\tau) = S_f\big(T - \frac{2\tau}{\sigma^2}\big),$$

$$\tilde{r} = \frac{2}{\sigma^2} r, \quad \widetilde{D}_0 = \frac{2}{\sigma^2} D_0, \quad \widetilde{T} = \frac{\sigma^2}{2} T.$$

The resulting forward–in–time equation then reads:

$$\frac{\partial \widetilde{V}}{\partial \tau} = S^2 \frac{\partial^2 \widetilde{V}}{\partial S^2} + (\tilde{r} - \widetilde{D}_0) S \frac{\partial \widetilde{V}}{\partial S} - \tilde{r}\, \widetilde{V}, \quad 0 < S < \widetilde{S}_f(\tau), \quad 0 \le \tau < \widetilde{T}, \tag{2.2a}$$

with the initial condition

$$\widetilde{V}(S,0) = (S-E)^+, \qquad 0 \le S < \widetilde{S}_f(0) = S_0, \tag{2.2b}$$

and the boundary conditions

$$\lim_{S \to 0} \widetilde{V}(S,\tau) = 0, \qquad 0 \le \tau \le \widetilde{T}, \tag{2.2c}$$

$$\widetilde{V}(\widetilde{S}_f(\tau),\tau) = (\widetilde{S}_f(\tau) - E)^+, \quad \frac{\partial \widetilde{V}}{\partial S}(\widetilde{S}_f(\tau),\tau) = 1, \qquad 0 \le \tau \le \widetilde{T}. \tag{2.2d}$$

The right hand side of (2.2a) is a well–known *Euler's differential equation* and therefore it is standard practice (cf. [29, § 4.1]) to transform (2.2a) to the heat equation. To do so, we let

$$\alpha = -\frac{1}{2}(\tilde{r} - \widetilde{D}_0 - 1), \quad \beta = -\alpha^2 - \tilde{r},$$

and use the change of variables

$$S = E e^x, \quad \widetilde{V}(S,\tau) = E e^{\alpha x + \beta \tau} v(x,\tau). \tag{2.3}$$

Then problem (2.2) is equivalent to the free boundary problem for the heat equation:

$$\frac{\partial v}{\partial \tau} = \frac{\partial^2 v}{\partial x^2}, \qquad -\infty < x < x_f(\tau), \quad 0 \le \tau < \widetilde{T}, \tag{2.4a}$$

where $x_f(\tau) = \ln(\widetilde{S}_f(\tau)/E)$. The equation (2.4a) is supplied with the initial condition

$$v(x,0) = g(x,0) = \bigl(e^{\frac{1}{2}(\tilde{r} - \widetilde{D}_0 + 1)x} - e^{\frac{1}{2}(\tilde{r} - \widetilde{D}_0 - 1)x}\bigr)^+, \qquad x < x_f(0), \tag{2.4b}$$

with $x_f(0) = \ln(\max(1, r/D_0))$ and the boundary conditions

$$\lim_{x \to -\infty} v(x,\tau) = 0, \qquad 0 \le \tau \le \widetilde{T}, \tag{2.4c}$$

$$v(x_f(\tau),\tau) = g(x_f(\tau),\tau), \qquad 0 \le \tau \le \widetilde{T}, \tag{2.4d}$$

$$e^{(\alpha-1)x + \beta\tau} \Bigl(\alpha v(x_f(\tau),\tau) + \frac{\partial v(x_f(\tau),\tau)}{\partial x}\Bigr) = 1, \qquad 0 \le \tau \le \widetilde{T}, \tag{2.4e}$$

where

$$g(x,\tau) = e^{-\alpha x - \beta \tau}(e^x - 1)^+,$$

It is well–known [24] that the free boundary $S_f(t)$ is a nondecreasing function and

$$S_f(T) \le S_f(t) \le S_f^*, \quad 0 \le t \le T, \tag{2.5}$$

with

$$S_f^* = \frac{\sqrt{-\beta} + \alpha}{\sqrt{-\beta} + \alpha - 1} E.$$

Thus if we set $x_f^* = \ln(S_f^*/E)$, then the free boundary $x_f(\tau)$ has the property [1]:

$$0 \le x_f(\tau) \le x_f^*, \quad 0 \le \tau \le \widetilde{T}. \tag{2.6}$$

Remark. We remark that the original Black–Scholes equation (2.1a) is degenerate at $S = 0$. However, the change of variables (2.3) transformed it into a uniformly parabolic initial boundary value problem (2.4).

3. The transparent boundary condition. The boundary problem (2.4) is posed on an unbounded and time–dependent domain $\Omega(\tau)$:

$$\Omega(\tau) = \{(x,\tau) \in \mathbb{R}^2 \,|\, x < x_f(\tau), \quad 0 \leq \tau \leq \widetilde{T}\}.$$

In the following we briefly present the derivation of the (analytic) TBC at the artificial boundary $x = a$. For this purpose we split the domain $\Omega(\tau)$ into the bounded time–dependent *interior domain*

$$\Omega_{int}(\tau) = \{(x,\tau) \in \mathbb{R}^2 \,|\, a < x < x_f(\tau), \quad 0 \leq \tau \leq \widetilde{T}\},$$

and the unbounded time–independent *exterior domain*

$$\Omega_{ext} = \{(x,\tau) \in \mathbb{R}^2 \,|\, x < a, \quad 0 \leq \tau \leq \widetilde{T}\}.$$

3.1. Derivation of the TBC. Here we determine the TBC at $x = a < 0$ such that the solution of the resulting initial boundary value problem coincides with the solution of the problem (2.4) restricted to Ω_{int}. For simplicity we assume that the initial data $v(x, 0)$ is compactly supported in the interior domain Ω_{int}, i.e. $g(x, 0) = 0$ for $x < a$. A strategy to overcome this restriction can be found in [11].

The analytic TBC for the heat equation was derived by several authors, e.g. [1], [15], [16]. Historically, this TBC was first derived by Papadakis [27] in the context of the Schrödinger equation. We remark that the derivation of the TBC for a parabolic convection diffusion equation with reaction term can be found in [10], [11].

For the derivation of the TBC at $x = a$ we consider the *interior problem*

$$\begin{aligned}
\frac{\partial v}{\partial \tau} &= \frac{\partial^2 v}{\partial x^2}, \qquad && (x,\tau) \in \Omega_{int}(\tau),\\
v(x,0) &= g(x,0), && a < x < x_f(0),\\
v_x(a,\tau) &= (T_a v)(a,\tau), && 0 \leq \tau \leq \widetilde{T},
\end{aligned} \tag{3.1}$$

together with the boundary conditions (2.4d), (2.4e) at the free boundary $x = x_f(\tau)$. We obtain the *Dirichlet–to–Neumann map* T_a by solving the *exterior problem*:

$$\begin{aligned}
\frac{\partial u}{\partial \tau} &= \frac{\partial^2 u}{\partial x^2}, \qquad && (x,\tau) \in \Omega_{ext},\\
u(x,0) &= 0, && x < a,\\
u(a,\tau) &= \Phi(\tau), && 0 \leq \tau \leq \widetilde{T}, \qquad \Phi(0) = 0,\\
u(-\infty,\tau) &= 0, && 0 \leq \tau \leq \widetilde{T},\\
(T_a\Phi)(\tau) &= u_x(a,\tau), && 0 \leq \tau \leq \widetilde{T}.
\end{aligned} \tag{3.2}$$

The problem on the exterior domain Ω_{ext} is coupled to the problem on the interior domain Ω_{int} by the assumption that v, v_x are continuous across the artificial boundary at $x = a$. One can solve (3.2) explicitly by the *Laplace–method*, i.e. we use the Laplace transformation of u

$$\hat{u}(x,s) = \int_0^\infty u(x,\tau)\, e^{-s\tau}\, d\tau,$$

where we set $s = \zeta + i\xi$, $\xi \in \mathbb{R}$, and $\zeta > 0$ is fixed, with the idea to later perform the limit $\zeta \to 0$. Now the exterior problem (3.2) is transformed to

$$\begin{aligned} &\hat{u}_{xx} - s\,\hat{u} = 0, \quad x < a, \\ &\hat{u}(a,s) = \hat{\Phi}(s). \end{aligned} \tag{3.3}$$

The solution to (3.3) which decays as $x \to -\infty$ is simply $\hat{u}(x,s) = \hat{\Phi}(s)\, e^{\sqrt[+]{s}(x-a)}$, $x < a$, where $\sqrt[+]{\ }$ denotes the branch of the square root with nonnegative real part. Consequently, the *transformed TBC* is:

$$\hat{u}_x(a,s) = \sqrt[+]{s}\,\hat{u}(a,s),$$

and after an inverse Laplace transformation (cf. [5]) the *TBC* at $x = a$ reads:

$$v_x(a,\tau) = \frac{1}{\sqrt{\pi}} \int_0^\tau \frac{v_\tau(a,\xi)}{\sqrt{\tau - \xi}}\, d\xi. \tag{3.4}$$

We observe that (3.4) has a weakly singular kernel and is a memory–type non–local function of τ, i.e. the computation of the solution at some time uses the solution at all previous times.

Remark. As noted in [16] the solution in Ω_{ext} can also be computed with

$$v(x,\tau) = -\frac{x-a}{2\sqrt{\pi}} \int_0^\tau e^{-\frac{(x-a)^2}{4(\tau-\xi)}} \frac{v(a,\xi)}{(\tau-\xi)^{3/2}}\, d\xi, \quad x < a. \tag{3.5}$$

Remark. The treatment of an *American put option* is completely analogous. Now one has to consider the Black–Scholes equation (2.1a) on the domain $S > S_f(t)$. The *terminal condition* at the expiry date $t = T$ then reads

$$V(S,T) = (E - S)^+, \qquad S > S_f(T), \tag{3.6a}$$

and the 'spatial' boundary conditions at $S = S_f(t)$, $S \to \infty$ are given by

$$V(S_f(t),t) = (E - S_f(t))^+, \quad \frac{\partial V}{\partial S}(S_f(t),t) = -1, \qquad 0 \le t \le T, \tag{3.6b}$$

$$\lim_{S\to\infty} V(S,t) = 0, \qquad 0 \le t \le T. \tag{3.6c}$$

Thus the TBC has to be constructed at $x = b$ with $b > S_f(t)$, for all $0 \le t \le T$.

3.2. Time–dependent parameters. It is possible to derive a TBC for American call options with time–varying interest rate $r = r(t)$, dividend yield $D = D(t)$ and volatility $\sigma = \sigma(t)$. This situation is more realistic but the time–dependence of the parameters $r = r(t)$ and $\sigma = \sigma(t)$ is unknown and must be modeled stochastically. In this case the Black–Scholes equation reads (cf. [32, §6.5])

$$\frac{\partial V}{\partial t} + \frac{1}{2}\sigma^2(t) S^2 \frac{\partial^2 V}{\partial S^2} + (r(t) - D(t)) S \frac{\partial V}{\partial S} - r(t) V = 0, \tag{3.7}$$

$0 < S < S_f(t)$, $0 \le t < T$. Making the substitutions

$$\bar{S} = S e^{\alpha(t)}, \quad \bar{V} = V e^{\beta(t)}, \quad \bar{t} = \gamma(t),$$

with

$$\alpha(t) = \int_t^T \big(r(\tau) - D(\tau)\big)\, d\tau, \quad \beta(t) = \int_t^T r(\tau)\, d\tau, \quad \gamma(t) = \int_t^T \sigma^2(\tau)\, d\tau,$$

then (3.7) becomes

$$\frac{\partial \bar{V}}{\partial \bar{t}} = \frac{1}{2}\bar{S}^2 \frac{\partial^2 \bar{V}}{\partial \bar{S}^2}, \qquad 0 < \bar{S} < \bar{S}_f(\bar{t}), \quad 0 \le \bar{t} \le \bar{T} = \gamma(0). \tag{3.8}$$

supplied with the initial condition $\bar{V}(\bar{S}, 0) = V(S, T)$ because $\gamma(T) = 0$. Since the right hand side of (3.8) is again of *Euler–type* one can proceed analogously to §3.1. The *Laplace–transformed exterior problem* reads:

$$\begin{aligned} &\frac{x^2}{2}\hat{u}_{xx} - s\,\hat{u} = 0, \quad x < a, \\ &\hat{u}(a, s) = \hat{\Phi}(s). \end{aligned} \tag{3.9}$$

The solution to (3.9) which decays as $x \to -\infty$ is simply

$$\hat{u}(x, s) = \hat{\Phi}(s)\, \left(\frac{x}{a}\right)^{(\frac{1}{2} - \frac{1}{2}\sqrt[+]{1+8s})}, \quad x < a,$$

and therefore the *transformed TBC* is:

$$\hat{u}_x(a, s) = a^{-1} \left(\frac{1}{2} - \sqrt{2}\sqrt[+]{s + \frac{1}{8}}\right) \hat{u}(a, s).$$

Finally an inverse Laplace transformation yields the desired *TBC* at $x = a$:

$$\bar{V}_x(a, \bar{t}) = \frac{\bar{V}(a, \bar{t})}{2a} - \frac{\sqrt{2}}{a\sqrt{\pi}} \int_0^{\bar{t}} \left(\bar{V}_{\bar{t}}(a, \xi) + \frac{\bar{V}(a, \xi)}{8}\right) \frac{e^{-(\bar{t}-\xi)/8}}{\sqrt{\bar{t} - \xi}}\, d\xi. \tag{3.10}$$

Remark. Most dividend payments on an index (e.g. the Dow Jones Industrial Average (DJIA) or the Standard and Poor's 500 (S&P500)) are so frequent that they can be modeled as a continuous payment. However, if companies make two or four payments per year then one has to treat the dividend payments discretely and the question is how to incorporate *discrete dividend payments* into the Black–Scholes equation. In the sequel we briefly review the results from [32]. We assume that there is only one dividend payment during the lifetime of the option at the *dividend date* t_d. Neglecting other factors like taxes, the asset price S must decrease exactly by the amount of the dividend payment d_0. Thus we have the *jump condition*

$$S(t_d^+) = (1 - d_0) S(t_d^-),$$

where t_d^-, t_d^+ denotes the moments just before and after t_d. This leads to the following effect on the option price

$$V(S, t_d^-) = V((1 - d_0)S, t_d^+), \tag{3.11}$$

i.e. the value of the option at S and time t_d^- is the same as the value immediately after the dividend date t_d but at the asset value $(1 - d_0)S$. To value a call option with one divident payment we solve the Black–Scholes equation from expiry $t = T$ until $t = t_d^+$ and use the relation (3.11) to compute the values at $t = t_d^-$. Finally, we continue to solve the Black–Scholes equation backwards starting at $t = t_d^-$ using these values as initial data. The transparent boundary conditions need not be modified for this case.

4. Discrete Transparent Boundary Conditions. In this section we shall address the question how to adequately discretize the analytic TBC (3.4) for a chosen full discretization of (2.4a) which in this example will be the Crank–Nicolson scheme. This scheme has been extremely popular for numerical solutions in finance since it is unconditionally stable and has second order accuracy in time and space. Furthermore it obeys a discrete maximum principle.

Instead of discretizing the analytic TBC (3.4) with its singularity our strategy is to derive the *discrete TBC* of the fully discretized problem. With the uniform grid points $x_j = a + j\Delta x$, $j = 0, 1, \dots$, $\tau_n = n\Delta\tau$, $n = 0, 1, \dots$ and the approximation $v_j^{(n)} \approx v(x_j, \tau_n)$ the *Crank–Nicolson scheme* for solving the heat equation (2.4a) is:

$$v_j^{(n+1)} - v_j^{(n)} = \rho \left(v_{j+1}^{(n+1/2)} - 2v_j^{(n+1/2)} + v_{j-1}^{(n+1/2)} \right), \tag{4.1}$$

with the abbreviation $v_j^{(n+1/2)} = (v_j^{(n+1)} + v_j^{(n)})/2$ and the *parabolic mesh ratio* $\rho = \Delta\tau/(\Delta x)^2$. While a uniform grid in x is necessary in the exterior domain, the interior grid may be nonuniform (e.g. logarithmic) in x. In the sequel we present different strategies to incorporate the analytic TBC (3.4) into the finite difference scheme (4.1).

4.1. Discretization strategies for the TBC. Here we want to compare three strategies to discretize the TBC (3.4) which is a rather delicate question with its mildly singular convolution kernel. First we review two known discretization techniques from Mayfield [22] and Han and Wu [16].

Discretized TBC of Mayfield. To compare our results we first review the *ad-hoc discretization strategy of Mayfield* applied to the heat equation (2.4a). According to the approach of Mayfield [22] for the Schrödinger equation, one way to discretize the analytic TBC (3.4), at $x = a$, in the equivalent form

$$v(a, \tau) = \frac{1}{\sqrt{\pi}} \int_0^\tau \frac{v_x(a, \xi)}{\sqrt{\tau - \xi}}\, d\xi \tag{4.2}$$

is

$$\begin{aligned}
\int_0^{\tau_n} \frac{v_x(a, \tau_n - \xi)}{\sqrt{\xi}}\, d\xi &\approx \frac{1}{\Delta x} \sum_{m=0}^{n-1} \big(v_1^{(n-m)} - v_0^{(n-m)}\big) \int_{\tau_m}^{\tau_{m+1}} \frac{d\xi}{\sqrt{\xi}} \\
&= \frac{2\sqrt{\Delta\tau}}{\Delta x} \sum_{m=0}^{n-1} \frac{\big(v_1^{(n-m)} - v_0^{(n-m)}\big)}{\sqrt{m+1} + \sqrt{m}}.
\end{aligned}$$

This approach leads to the following *discretized TBC* for the heat equation:

$$v_1^{(n)} - v_0^{(n)} = \frac{\sqrt{\pi}\Delta x}{2\sqrt{\Delta\tau}} v_0^{(n)} - \sum_{m=1}^{n-1} \tilde{\ell}^{(m)} \big(v_1^{(n-m)} - v_0^{(n-m)}\big), \tag{4.3}$$

with the convolution coefficients given by

$$\tilde{\ell}^{(m)} = \frac{1}{\sqrt{m+1} + \sqrt{m}}. \tag{4.4}$$

Discretized TBC of Han and Wu. Recently a very similar discretization strategy was introduced in [16]. The authors discretized the analytic TBC (3.4) in the following way

$$\begin{aligned}\int_0^{\tau_n} \frac{v_\tau(a,\xi)}{\sqrt{\tau_n-\xi}}\,d\xi &\approx \sum_{m=0}^{n-1} v_\tau(a,\xi_m)\int_{\tau_m}^{\tau_{m+1}} \frac{d\xi}{\sqrt{\tau_n-\xi}}\\ &= 2\Delta\tau \sum_{m=0}^{n-1} \frac{v_\tau(a,\xi_m)}{\sqrt{\tau_n-\tau_{m+1}}+\sqrt{\tau_n-\tau_m}}.\end{aligned}$$

This approach leads to the condition

$$v_1^{(n)} - v_{-1}^{(n)} = \frac{4}{\sqrt{\pi}}\frac{1}{\sqrt{\rho}} \sum_{m=1}^{n} \frac{v_0^{(m)}-v_0^{(m-1)}}{\sqrt{n-m}+\sqrt{n-m+1}}. \tag{4.5}$$

By applying a purely implicit scheme to the heat equation at the artificial boundary $x_0 = a$, i.e.

$$v_0^{(n)} - v_0^{(n-1)} = \rho\left(v_1^{(n)} - 2v_0^{(n)} + v_{-1}^{(n)}\right),$$

one can eliminate the fictitious value $v_{-1}^{(n)}$ in (4.5) to obtain the *discretized TBC of Han and Wu* [16]:

$$(1+2\rho+B)\,v_0^{(n)} - 2\rho\,v_1^{(n)} = (1+B)\,v_0^{(n-1)} - B\sum_{m=1}^{n-1} \tilde{\ell}^{(n-m)}\left(v_0^{(m)} - v_0^{(m-1)}\right), \tag{4.6}$$

with the abbreviation $B = 4\sqrt{\rho}/\sqrt{\pi}$ and the convolution coefficients given in (4.4).

On the fully discrete level the discretized TBCs like (4.3), (4.6) are not exactly transparent any more and can lead to an unstable numerical scheme. This was proven for a discretized TBC of the form (4.3) by Mayfield [22] in the case of the Schrödinger equation.

The discrete transparent boundary condition. In order to avoid any numerical reflections at the artificial boundary and to ensure unconditional stability of the resulting scheme we will construct in the next subsection a *discrete TBC* instead of choosing an ad–hoc discretization of the analytic TBC (3.4) like Mayfields approach [22] or the approach of Han and Wu [16]. The discrete TBC completely avoids any numerical reflections at the boundary at no additional computational costs (compared to ad–hoc discretization strategies like (4.3), (4.6)).

4.2. Derivation of the DTBC. We mimic the derivation from §3 on a purely discrete level: we obtain the DTBC by solving the *discrete exterior problem*, i.e. (4.1) for $j \le 1$.

We apply for j fixed the Z–transformation:

$$\mathcal{Z}\{v_j^{(n)}\} = \hat{v}_j(z) := \sum_{n=0}^{\infty} v_j^{(n)}\,z^{-n}, \quad |z| > R_{\hat{v}_j},$$

($R_{\hat{v}_j}$ denotes the convergence radius of the Laurent series) to solve (4.1) for $j \le 1$ explicitly. Again we assume for the initial data, $v_j^{(0)} = 0,\ j \le 1$ and obtain the *transformed exterior scheme*

$$\frac{2}{\rho}\frac{z-1}{z+1}\,\hat{v}_j(z) = \hat{v}_{j+1} - 2\hat{v}_j + \hat{v}_{j-1}, \quad j \le 1. \tag{4.7}$$

The two linearly independent solutions of the resulting *second order difference equation* (4.7) take the form

$$\hat{v}_j(z) = (\nu_{1,2})^{j+1}(z), \quad j \leq 1,$$

where $\nu_{1,2}(z)$ are the solutions of the quadratic equation

$$\nu^2 - 2\Big[1 + \frac{1}{\rho}\frac{z-1}{z+1}\Big]\nu + 1 = 0.$$

Since we are seeking decreasing modes as $j \to -\infty$ we have to require $|\nu_1| > 1$ and obtain the Z–transformed *discrete TBC* as

$$\hat{v}_1(z) = \nu_1(z)\,\hat{v}_0(z). \tag{4.8}$$

It only remains to calculate the inverse Z–transform of $\nu_1(z)$ to obtain the discrete TBC from (4.8). In a tedious calculation this can be performed explicitly (cf. [11]) and the discrete TBC becomes:

$$v_1^{(n)} = \ell^{(n)} * v_0^{(n)} = \sum_{k=1}^{n} \ell^{(n-k)} v_0^{(k)}, \quad n \geq 1, \tag{4.9}$$

with convolution coefficients $\ell^{(n)}$ given in [11]. Since the asymptotical behaviour $\ell^{(n)} \sim 4(-1)^n/\rho$ of the convolution coefficients may lead to subtractive cancellation in (4.9) we prefer to use the following *summed coefficients* in the implementation

$$s^{(n)} := \ell^{(n)} + \ell^{(n-1)}, \quad n \geq 1, \quad s^{(0)} := \ell^{(0)}. \tag{4.10}$$

The DTBC then reads

$$v_1^{(n)} - s^{(0)} v_0^{(n)} = \sum_{k=1}^{n-1} s^{(n-k)} v_0^{(k)} - v_1^{(n-1)}, \quad n \geq 1, \tag{4.11}$$

with the convolution coefficients

$$\begin{aligned} s^{(0)} &= 1 + \frac{1+\sqrt{1+2\rho}}{\rho}, \quad s^{(1)} = 1 - \frac{1}{\rho} - \frac{1}{\rho\sqrt{1+2\rho}}, \\ s^{(n)} &= -\frac{\sqrt{1+2\rho}}{\rho}\,\frac{\widetilde{P}_n(\mu) - \lambda^{-2}\widetilde{P}_{n-2}(\mu)}{2n-1}, \quad n \geq 2, \end{aligned} \tag{4.12}$$

where $\widetilde{P}_n(\mu) := \lambda^{-n} P_n(\mu)$ denotes the *"damped" Legendre polynomials* ($\widetilde{P}_0 \equiv \lambda^{-1}$, $\widetilde{P}_{-1} \equiv 0$). The parameters λ, μ are given by

$$\lambda = \frac{\sqrt{1+2\rho}}{\sqrt[+]{1-2\rho}}, \qquad \mu = \frac{1}{\sqrt{1+2\rho}\,\sqrt[+]{1-2\rho}}.$$

Alternatively, the convolution coefficients can be computed by the recursion formula

$$s^{(n+1)} = \frac{2n-1}{n+1}\mu\lambda^{-1}s^{(n)} - \frac{n-2}{n+1}\lambda^{-2}s^{(n-1)}, \quad n \geq 2, \tag{4.13}$$

which can be used after calculating $s^{(n)}$, $n = 0, 1, 2$ by the formula (4.12).

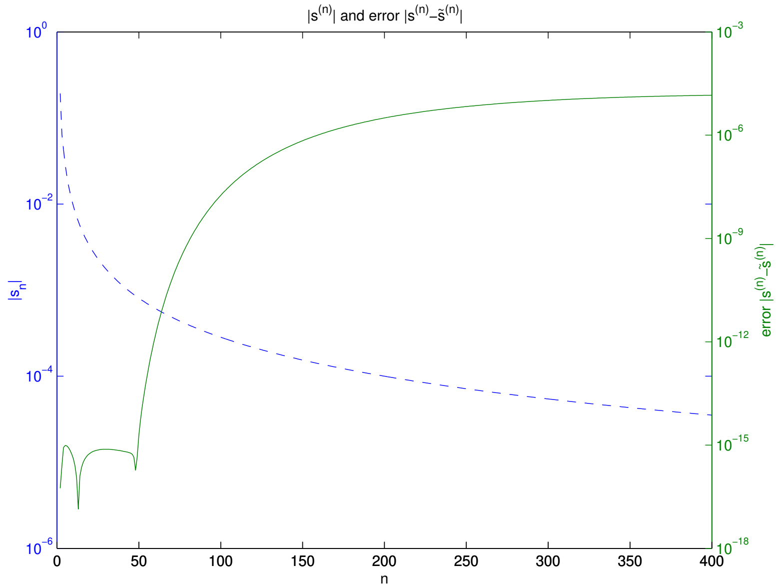

FIG. 4.1. *Convolution coefficients* $s^{(n)}$ (4.12) *(left axis, dashed line) and error* $|s^{(n)} - \tilde{s}^{(n)}|$ *of the approximated convolution coefficients* (5.1) *(right axis, solid line);* $\rho = 1$, $L = 20$.

In Fig. 4.1 the values of the summed coefficients $s^{(n)}$ are presented in a logarithmic plot. One clearly observes their rapid decay property $s^{(n)} = \mathrm{O}(n^{-3/2})$ [11] which motivates a *simplified discrete TBC* by restricting (4.11) to a convolution over the "recent past" (last M time levels):

$$v_1^{(n)} - s^{(0)} v_0^{(n)} = \sum_{k=n-M}^{n-1} s^{(n-k)} v_0^{(k)} - v_1^{(n-1)}, \quad n \geq 1, \tag{4.14}$$

We note that the stability of the resulting scheme is still not proven yet.

For a concise discussion of several discretization strategies of analytic TBCs, the derivation of the DTBC for a class of difference schemes for a general convection diffusion equation and a stability proof of the recursion formula (4.13) we refer to [11].

5. Approximation by Sums of Exponentials. An ad-hoc implementation of the discrete convolution (4.11), with convolution coefficients $s^{(n)}$ from (4.12), has still one disadvantage. The boundary condition is non–local in time and therefore computationally expensive. In fact, the evaluation of (4.11) is as expensive as for the discretized TBCs (4.3), (4.6). As a remedy, we proposed in [3] the sum-of-exponentials ansatz. In the work to come, we briefly review this approach.

In order to derive a fast numerical method to calculate the discrete convolution in (4.11), we approximate the coefficients $s^{(n)}$ by the following (*sum of exponentials*):

$$s^{(n)} \approx \tilde{s}^{(n)} := \begin{cases} s^{(n)}, & n = 0, 1 \\ \displaystyle\sum_{l=1}^{L} b_l \, q_l^{-n}, & n = 2, 3, \dots, \end{cases} \tag{5.1}$$

where $L \in \mathbb{N}$ is a fixed number. Note that the approximation properties of $\tilde{s}^{(n)}$ depend on L, and the corresponding set $\{b_l, q_l\}$. Below we propose a deterministic method of finding $\{b_l, q_l\}$ for fixed L.

The "split" definition of $\{\tilde{s}^{(n)}\}$ in (5.1) is motivated by the different nature of the first two coefficients in (4.12). Including them into the discrete sum-of-exponential would then yield less accurate approximation results.

Let us fix L and consider the formal power series:

$$f(x) := s^{(2)} + s^{(3)}x + s^{(4)}x^2 + \dots, \quad |x| \le 1. \tag{5.2}$$

If there exists the $[L-1|L]$ *Padé approximation*

$$\tilde{f}(x) := \frac{P_{L-1}(x)}{Q_L(x)}$$

of (5.2), then its Taylor series

$$\tilde{f}(x) = \tilde{s}^{(2)} + \tilde{s}^{(3)}x + \tilde{s}^{(4)}x^2 + \dots$$

satisfies the conditions

$$\tilde{s}^{(n)} = s^{(n)}, \qquad n = 2, 3, \dots, 2L+1, \tag{5.3}$$

due to the definition of the Padé approximation rule.

THEOREM 5.1 ([3]). *Let $Q_L(x)$ have L simple roots q_l with $|q_l| > 1$, $l = 1, \dots, L$. Then*

$$\tilde{s}^{(n)} = \sum_{l=1}^{L} b_l\, q_l^{-n}, \qquad n = 2, 3, \dots, \tag{5.4}$$

where

$$b_l := -\frac{P_{L-1}(q_l)}{Q'_L(q_l)}\, q_l \neq 0, \qquad l = 1, \dots, L. \tag{5.5}$$

It follows from (5.3) and (5.4) that the set $\{b_l, q_l\}$ defined in Theorem 5.1 can be used in (5.1) at least for $n = 2, 3, .., 2L+1$. The main question now is: Is it possible to use these $\{b_l, q_l\}$ also for $n > 2L+1$? In other words, how good is the approximation

$$\tilde{s}^{(n)} \approx s^{(n)}, \qquad n > 2L+1.$$

The above analysis permits us to give the following description of the approximation to the convolution coefficients $s^{(n)}$ by the representation (5.1) if we use a $[L-1|L]$ Padé approximant for (5.2): the first $2L$ coefficients are reproduced exactly, see (5.3); however, the asymptotic behaviour of $s^{(n)}$ and $\tilde{s}^{(n)}$ (as $n \to \infty$) differs strongly (algebraic versus exponential decay). A typical graph of $|s^{(n)} - \tilde{s}^{(n)}|$ versus n for $L = 20$ is shown in Fig. 4.1.

So far we have discussed how to calculate and approximate the DTBC for one *fixed* discretization. However, a nice property of this approach consists of the following: once the approximate convolution coefficients $\{\tilde{s}^{(n)}\}$ are calculated for a particular mesh ratio ρ, it is easy to transform them into appropriate coefficients for any mesh ratio ρ_*.

THEOREM 5.2 ([3]). *Let a rational function*

$$\hat{\tilde{s}}(z) := s^{(0)} + \frac{s^{(1)}}{z} + \sum_{l=1}^{L} \frac{b_l}{q_l z - 1} \tag{5.6}$$

approximate the Z-transform of the convolution kernel $\{s^{(n)}\}_{n=0}^{\infty}$ *corresponding to a DTBC for the equation* (4.1) *with a given mesh ratio* ρ *(*$\hat{\tilde{s}}$ *is the Z-transform of* $\{\tilde{s}^{(n)}\}$ *from* (5.1)*). Then, for another mesh ratio* $\rho_\star$*, one can take the approximation*

$$\hat{\tilde{s}}_\star(z) := s_\star^{(0)} + \frac{s_\star^{(1)}}{z} + \sum_{l=1}^{L} \frac{b_l^\star}{q_l^\star z - 1}, \tag{5.7}$$

where

$$\begin{aligned} s_\star^{(0)} &:= \hat{\tilde{s}}(a/b) \quad (:= s^{(0)} \textit{ if } b = 0), \\ b_l^\star &:= b_l q_l \frac{a^2 - b^2}{(a - q_l b)(q_l a - b)} \frac{1 + q_l^\star}{1 + q_l}, \qquad q_l^\star := \frac{q_l a - b}{a - q_l b}, \\ a &:= (\frac{1}{\rho} + \frac{1}{\rho_\star}), \qquad b := (\frac{1}{\rho} - \frac{1}{\rho_\star}). \end{aligned} \tag{5.8}$$

While the Padé–algorithm provides a method to calculate approximate convolution coefficients $\tilde{s}^{(n)}$ for a *fixed mesh ratio* ρ, this transformation rule yields the natural link between *different mesh ratios* $\rho_\star$ (and L fixed).

Example. For $L = 20$ we calculated the coefficients $\{b_l, q_l\}$ with the mesh ratio $\rho = 1$ and then used the Transformation rule 5.2 to calculate the coefficients $\{b_l^*, q_l^*\}$ for the mesh ratio $\rho_\star = 0.8$. Fig. 5.1 shows that the resulting convolution coefficients $\tilde{s}_*^{(n)}$ are in this example even better approximations to the exact coefficients $s^{(n)}$ than the coefficients $\tilde{s}^{(n)}$, which are obtained directly from the Padé algorithm discussed in Theorem 5.1. Hence, the numerical solution of the corresponding heat equation is also more accurate.

5.1. Fast Evaluation of the Discrete Convolution.. Let us consider the approximation (5.1) of the discrete convolution kernel appearing in the DTBC (4.11). With these "exponential" coefficients the convolution

$$C^{(n)} := \sum_{m=1}^{n-1} \tilde{s}^{(n-m)} v_0^{(m)}, \qquad \tilde{s}^{(n)} = \sum_{l=1}^{L} b_l\, q_l^{-n}, \tag{5.9}$$

where $|q_l| > 1$, of a discrete function $v_0^{(m)}$, $m = 1, 2, \ldots$, with the kernel coefficients $\tilde{s}^{(n)}$, can be calculated by recurrence formulas, and this will reduce the numerical effort significantly.

A straightforward calculation (cf. [3]) yields: The value $C^{(n)}$, from (5.9) for $n \geq 2$, can be represented by

$$C^{(n)} = \sum_{l=1}^{L} C_l^{(n)}, \tag{5.10}$$

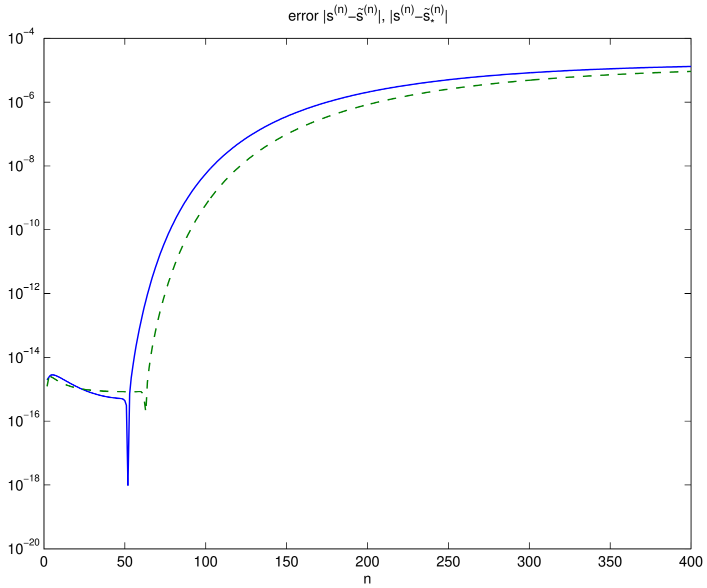

FIG. 5.1. *Approximation error of the approximate convolution coefficients for $\rho = 0.8$: The error of $\tilde{s}_*^{(n)}$ (- - -) obtained from the transformation rule and the error of $\tilde{s}^{(n)}$ (—) obtained from a direct Padé approximation of the exact coefficients $s^{(n)}$.*

where

$$C_l^{(1)} \equiv 0,$$

$$C_l^{(n)} = q_l^{-1} C_l^{(n-1)} + b_l\, q_l^{-1} v_0^{(n-1)}, \qquad n = 2, 3, \ldots, \quad l = 1, \ldots, L. \tag{5.11}$$

In summary we now list the steps of the proposed method to evaluate an approximate DTBC:

1. Prescribe L in (5.1), take $\rho = 1$, and calculate $s^{(n)}, n = 0, \ldots, 2L+1$, by formula (4.12).

2. Use the $[L-1|L]$–Padé algorithm for the series (5.2) with $\tilde{s}^{(n)} := s^{(n)}$, $n = 2, 3, \ldots, 2L+1$ in order to find $\{b_l, q_l\}$ for (5.1) in accordance with Theorem 5.1.

The steps 1. and 2. are made once and for all; see Appendix with the table of coefficients for $L = 5$, 10.

3. For given ratio $\rho_\star$, use formulas (5.8), with $\rho = 1$ and $\{b_l, q_l\}$ from step 2, for the calculation of $\{b_l^\star, q_l^\star\}$.

4. Implement the recurrence formulas (5.10)–(5.11) to calculate the approximate convolutions in (4.11). The coefficients $s_*^{(0)}$, $s_*^{(1)}$ have to be calculated by use of (4.12).

We remark that the Padé approximation must be performed with high precision ($2L-1$ digits mantissa length) to avoid a 'nearly breakdown' by ill conditioned steps in the Lanczos algorithm. If such problems still occur or if one root of the denominator is smaller than 1 in absolute value, the orders of the numerator and denominator polynomials are successively reduced.

6. Numerical treatment of the free boundary. In this section we shall describe briefly how to treat numerically the free boundary $x_f(\tau)$ in (2.4). For more details on the optimal exercise time we refer the reader to [4].

Up to now no exact analytical formula for the free boundary profile $x_f(\tau)$ in (2.4) is known but several authors derived approximate expressions for valuing American call and put options, e.g. [14]. Recently, in a promising approach [28], Ševčovič obtained a semi–explicit formula for an American call in the case $r > D_0$. By transforming (2.1) to a nonlinear parabolic equation on a fixed domain and applying Fourier sine and cosine transformations he derived a nonlinear singular integral equation determining the shape of the free boundary. This integral equation can be solved effectively by means of successive iterations.

However, since the Black–Scholes equation (2.1a) couples $V(S,t)$ to $S_f(t)$ we prefer to determine the option value numerically in connection with the free boundary. To do this, many different numerical methods are developed, e.g. the standard method consists in the reformulation to a linear complementary problem and solution by the projected SOR method of Cryer [9]. Alternatively, penalty and front–fixing methods were developed (e.g. in [13], [25]). A disadvantage of these methods is the change of the underlying model. A different approach [17] is based on a recursive calculation of the early exercise boundary, estimating the boundary only at some points and then approximating the whole boundary by Richardson extrapolation. Explicit boundary tracking algorithms are e.g. a finite difference bisection scheme [21] or the *front–tracking strategy of Han and Wu* [16]. In this work we will use the later approach of Han and Wu, which will be described now briefly.

In [16] the authors applied the strong maximum principle for parabolic equations to the Black–Scholes equation for the derivative $\widetilde{V}_S$ and the equation (2.2a) extended to the time–independent domain $S > 0$ (which is known in the literature as the *Jamshidian equation* [18]). The outcome is a very useful inequality [16, Eq. (30] for the numerical determination of the location of the free boundary $x_f(\tau)$: for a given τ the free boundary is the only point that fulfils both the equation (2.4a) and the high contact condition $V_S(S,t) = 1$, i.e. (2.4e). If the boundary condition $v(x,\tau) = g(x,\tau)$ is posed at some point $x > x_f(\tau)$ then $v(x,\tau) < g(x,\tau)$ will occur for some $x < x_f(\tau)$. To solve the Crank–Nicolson scheme (4.1) Han and Wu used the common *Thomas algorithm* [31] for the arising tridiagonal system. Once the boundary condition

$$v_{J+1}^{(n+1)} = g_{J+1}^{(n+1)}, \tag{6.1}$$

with $g_J^{(n)} = g(x_J, \tau_n)$, is given at some grid point x_{J+1} then the backward sweep of the Thomas algorithm calculates the solution $v_j^{(n+1)}$ for all $0 \le j \le J$. The index J is simply the largest index such that

$$v_J^{(n+1)} \ge g_J^{(n+1)} \tag{6.2}$$

holds.

Remark. For the American call (in contrast to the American put) it is possible to derive a series for the location of the optimal exercise boundary close to expiry using standard asymptotic analysis (cf. [2], [32]). This local analysis of the free boundary $S_f(t)$ yields

$$S_f(t) \sim S_f(T)\left(1 + \xi_0\sqrt{\frac{1}{2}\sigma^2(T-t)} + \dots\right), \text{ as } t \to T, \tag{6.3}$$

where $\xi_0 = 0.9034\ldots$ is a 'universal' constant of call option pricing. Equation (6.3) can be rewritten as

$$x_f(\tau) \sim \ln\left[\frac{S_f(T)}{E}\left(1+\xi_0\sqrt{\tau}+\ldots\right)\right], \text{ as } \tau \to 0. \tag{6.4}$$

With only a very few terms one gets a fairly accurate result and thus (6.4) will serve us as a check of the above mentioned tracking strategy of Han and Wu. Note that this result is especially useful in the first time levels of a numerical calculation where rapid changes in $x_f(\tau)$ influence the whole solution region.

7. Stability analysis of the artificial boundary condition. Here we analyze the stability of the Crank–Nicolson scheme (4.1) along with the DTBC (4.11) or its approximated version. Since we will focus on the fact that the (approximated) DTBC does not destroy the unconditional stability of the underlying finite difference scheme, we consider the following problem on the half–space $j \geq 0$:

$$\begin{cases} v_j^{(n+1)} - v_j^{(n)} &= \rho\left(v_{j+1}^{(n+1/2)} - 2v_j^{(n+1/2)} + v_{j-1}^{(n+1/2)}\right), \quad j \geq 1, \\ v_j^{(0)} &= g(x_j,0), \quad j = 0,1,2,\ldots \\ \text{with } v_0^{(0)} &= v_1^{(0)} = 0, \\ \hat{v}_1(z) &= \hat{\ell}(z)\hat{v}_0(z), \end{cases} \tag{7.1}$$

where the transformed boundary kernel $\hat{\ell}(z) = \nu_1(z)$ is given by (4.8). In the sequel we want to bound the exponential growth of solutions to the numerical scheme (7.1) for a fixed mesh ratio. We will prove an estimate of the discrete solution to (7.1) in the discrete ℓ^2–norm:

$$\|v^{(n)}\|_2^2 := \Delta x \sum_{j=1}^{\infty} |v_j^{(n)}|^2. \tag{7.2}$$

THEOREM 7.1 (Growth condition). *Let the transformed boundary kernel $\hat{\ell}$ satisfy*

$$\text{Re } \hat{\ell}(\beta e^{i\varphi}) \geq 1, \quad \forall\, 0 \leq \varphi \leq 2\pi, \tag{7.3}$$

for some (sufficiently large) $\beta \geq 1$. Assume also that $\hat{\ell}(z)$ is analytic for $|z| \geq \beta$. Then, the solution of (7.1) *satisfies the a-priori estimate in the discrete ℓ^2–norm:*

$$\|v^{(n+1)}\|_2 \leq \beta^n\left(\|v^{(0)}\|_2 + \sqrt{\frac{(\beta-1)\rho}{2}}\|\Delta^- v^{(0)}\|_2\right), \quad n \in \mathbb{N}_0. \tag{7.4}$$

Proof. The proof is based on a discrete energy estimate for the new variable

$$u_j^{(n)} := v_j^{(n)}\,\beta^{-n},$$

which fulfills

$$\beta^{-n}\left(v_j^{(n+1)} \pm v_j^{(n)}\right) = u_j^{(n+1)} \pm u_j^{(n)} + (\beta-1)u_j^{(n+1)},$$

and therefore satisfies

$$u_j^{(n+1)} - u_j^{(n)} = \rho\left(u_{j+1}^{(n+1/2)} - 2u_j^{(n+1/2)} + u_{j-1}^{(n+1/2)}\right) \tag{7.5a}$$
$$+ (\beta-1)\Big[\frac{\rho}{2}\left(u_{j+1}^{(n+1)} - 2u_j^{(n+1)} + u_{j-1}^{(n+1)}\right) - u_j^{(n+1)}\Big], \quad j \geq 1$$

$$u_j^{(0)} = v_j^{(0)}, \quad j = 0,1,2\ldots, \tag{7.5b}$$

$$\Delta^+\hat{u}_0(z) = \left(\hat{\ell}(\beta z) - 1\right)\hat{u}_0(z). \tag{7.5c}$$

The transformed discrete TBC (7.5c) can be written in physical space as

$$\Delta^+ u_0^{(n)} = \frac{\tilde\ell^{(n)}}{\beta^n} * u_0^{(n)} = \sum_{m=0}^{n} \Bigl(\tilde\ell^{(n-m)}\,\beta^{m-n}\Bigr)\, u_0^{(m)},$$

where $\tilde\ell^{(n)} := \ell^{(n)} - \delta_n^0$ is given in (4.9) and $\Delta^+ u_0^{(n)} = u_1^{(n)} - u_0^{(n)}$ denotes the usual forward difference. First we multiply (7.5a) by $u_j^{(n)}/\beta$ and then by $u_j^{(n+1)}$:

$$\begin{aligned} u_j^{(n)}\Bigl(u_j^{(n+1)} - u_j^{(n)}\Bigr) &= \rho u_j^{(n)}\Bigl(u_{j+1}^{(n+1/2)} - 2u_j^{(n+1/2)} + u_{j-1}^{(n+1/2)}\Bigr) \\ &\quad - \beta^{-1}(\beta-1)u_j^{(n)}\bigl[\frac{\rho}{2}\bigl(u_{j+1}^{(n)} - 2u_j^{(n)} + u_{j-1}^{(n)}\bigr) + u_j^{(n)}\bigr], \end{aligned} \tag{7.6a}$$

$$\begin{aligned} u_j^{(n+1)}\Bigl(u_j^{(n+1)} - u_j^{(n)}\Bigr) &= \rho u_j^{(n+1)}\Bigl(u_{j+1}^{(n+1/2)} - 2u_j^{(n+1/2)} + u_{j-1}^{(n+1/2)}\Bigr) \\ &\quad + (\beta-1)u_j^{(n+1)}\bigl[\frac{\rho}{2}\bigl(u_{j+1}^{(n+1)} - 2u_j^{(n+1)} + u_{j-1}^{(n+1)}\bigr) - u_j^{(n+1)}\bigr]. \end{aligned} \tag{7.6b}$$

Note that we used equation (7.5a) to modify the last term of (7.6a). Next we add (7.6a) and (7.6b), sum it up for the range $j = 1, 2, \ldots$ and obtain using the summation by parts rule:

$$\begin{aligned} \sum_{j=1}^{\infty}\bigl[(u_j^{(n+1)})^2 - (u_j^{(n)})^2\bigr] &= -2\rho\sum_{j=1}^{\infty}(\Delta^- u_j^{(n+1/2)})^2 \\ &\quad - (\beta-1)\frac{\rho}{2}\sum_{j=1}^{\infty}(\Delta^- u_j^{(n+1)})^2 + \frac{\beta-1}{\beta}\frac{\rho}{2}\sum_{j=1}^{\infty}(\Delta^- u_j^{(n)})^2 \\ &\quad - (\beta-1)\sum_{j=1}^{\infty}(u_j^{(n+1)})^2 - \frac{\beta-1}{\beta}\sum_{j=1}^{\infty}(u_j^{(n)})^2 \\ &\quad - \frac{\rho}{2\beta}(u_0^{(n)} + \beta u_0^{(n+1)})\Delta^+(u_0^{(n)} + \beta u_0^{(n+1)}), \end{aligned} \tag{7.7}$$

where $\Delta^- u_j^{(n)} = u_j^{(n)} - u_{j-1}^{(n)}$ denotes the backward difference. Now summing (7.7) from time level $n = 0$ to $n = N$ yields:

$$\begin{aligned} \beta\|u^{(N+1)}\|_2^2 = \beta^{-1}\|u^{(0)}\|_2^2 &- \frac{(\beta^2-1)}{\beta}\sum_{n=1}^{N}\|u^{(n)}\|_2^2 \\ &- 2\rho\sum_{n=0}^{N}\|\Delta^- u^{(n+1/2)}\|_2^2 - \frac{(\beta-1)^2}{\beta}\frac{\rho}{2}\sum_{n=1}^{N}\|\Delta^- u^{(n)}\|_2^2 \\ &+ \frac{(\beta-1)}{\beta}\frac{\rho}{2}\|\Delta^- u^{(0)}\|_2^2 - (\beta-1)\frac{\rho}{2}\|\Delta^- u^{(N+1)}\|_2^2 \\ &- \frac{\rho}{2\beta}\sum_{n=0}^{N}(u_0^{(n)} + \beta u_0^{(n+1)})\Delta^+(u_0^{(n)} + \beta u_0^{(n+1)}). \end{aligned} \tag{7.8}$$

Noting that $\beta \geq 1$, we obtain from (7.8) the following estimate:

$$\begin{aligned} \|u^{(N+1)}\|_2^2 \leq \beta^{-2}\|u^{(0)}\|_2^2 &+ \frac{(\beta-1)}{\beta^2}\frac{\rho}{2}\|\Delta^- u^{(0)}\|_2^2 \\ &- \frac{\rho}{2\beta^2}\sum_{n=0}^{N}(u_0^{(n)} + \beta u_0^{(n+1)})\Delta^+(u_0^{(n)} + \beta u_0^{(n+1)}). \end{aligned} \tag{7.9}$$

It remains to show that the boundary–memory–term in (7.9) is of *positive type*. To this end we define (for N fixed) the two sequences,

$$g^{(n)} := \begin{cases} u_0^{(n)} + \beta u_0^{(n+1)}, & n = 0, \dots, N, \\ 0, & n > N, \end{cases}$$

$$f^{(n)} := \frac{\tilde{\ell}^{(n)}}{\beta^n} * g^{(n)} = \sum_{m=0}^{n} \frac{\tilde{\ell}^{(n-m)}}{\beta^{n-m}}\, g^{(m)}, \quad n \in \mathbb{N}_0,$$

i.e. $\sum_{n=0}^N f^{(n)}\, g^{(n)} \geq 0$ is to show. The Z–transform $\mathcal{Z}\{f^{(n)}\} = \hat{f}(z)$ is analytic for $|z| > 0$, since it is a finite sum. The Z–transform $\mathcal{Z}\{f^{(n)}\}$ then satisfies $\hat{f}(z) = (\hat{\ell}(\beta z) - 1)\hat{g}(z)$ and is analytic for $|z| \geq 1$. Using Plancherel's Theorem for Z–transforms we have

$$\begin{aligned} \sum_{n=0}^{N} f^{(n)} g^{(n)} &= \frac{1}{2\pi}\int_0^{2\pi} \hat{f}(e^{i\varphi})\overline{\hat{g}(e^{i\varphi})}\, d\varphi = \frac{1}{\pi}\int_0^{\pi} \mathrm{Re}\left\{\hat{f}(e^{i\varphi})\,\overline{\hat{g}(e^{i\varphi})}\right\} d\varphi \\ &= \frac{1}{\pi}\int_0^{\pi} |\hat{g}(e^{i\varphi})|^2\big(\mathrm{Re}\left\{\hat{\ell}(\beta e^{i\varphi})\right\} - 1\big)\, d\varphi, \end{aligned} \tag{7.10}$$

where we have used the fact that $\hat{f}(\bar{z}) = \overline{\hat{f}(z)}$, $\hat{g}(\bar{z}) = \overline{\hat{g}(z)}$, since $f_n, g_n \in \mathbb{R}$. Using (7.10) for the boundary term in (7.9) now gives:

$$\begin{aligned} \|u^{(N+1)}\|_2^2 \leq \beta^{-2}\|u^{(0)}\|_2^2 &+ \frac{(\beta-1)}{\beta^2}\frac{\rho}{2}\|\Delta^- u^{(0)}\|_2^2 \\ &- \frac{\rho}{2\pi\beta^2}\int_0^{\pi} |(1+\beta e^{i\varphi})\hat{u}_0(e^{i\varphi})|^2\big(\mathrm{Re}\left\{\hat{\ell}(\beta e^{i\varphi})\right\} - 1\big)\, d\varphi. \end{aligned}$$

Our assumption on $\hat{\ell}$ therefore implies

$$\|u^{(N+1)}\|_2 \leq \beta^{-1}\|u^{(0)}\|_2 + \frac{\sqrt{\beta-1}}{\beta}\sqrt{\frac{\rho}{2}}\|\Delta^- u^{(0)}\|_2, \quad \forall\, N \geq 0,$$

and the result of the theorem follows. ∎

Example: The exact DTBC. For the case of the exact discrete DTBC the assumption of Theorem 7.1 can easily be checked: This property of $\hat{\ell}$ can be shown for $\beta = 1$ in the following way. On the unit circle $z = e^{i\varphi}$, $0 \leq \varphi \leq 2\pi$, we have

$$y(z) := \frac{1}{\rho}\Big(\frac{z-1}{z+1}\Big) = \frac{1}{\rho}\Big(i \tan\frac{\varphi}{2}\Big), \qquad 0 \leq \varphi \leq 2\pi.$$

Therefore we obtain the requested property

$$\mathrm{Re}\,\{\hat{\ell}(z)\} = 1 + \mathrm{Re}\left\{ \sqrt[+]{y(z)\big(2 + y(z)\big)}\ \right\} \geq 1,$$

for $z = e^{i\varphi}$, $0 \leq \varphi \leq 2\pi$, i.e. for the exact discrete TBC we have the estimate

$$\|v^{(n)}\|_2 \leq \|v^{(0)}\|_2, \quad n \in \mathbb{N}. \tag{7.11}$$

Remark. Above we have assumed that the Z–transformed boundary kernel $\hat{\ell}(z)$ is analytic for $|z| \geq \beta$. Hence its real part is a harmonic function there. Since the average of $\hat{\ell}(z)$ on the circles $z = \beta e^{i\varphi}$ equals $\ell^{(0)} = \hat{\ell}(z = \infty)$, condition (7.3) implies $\operatorname{Re} \hat{\ell}(z = \infty) \geq 1$. Then we have the following simple consequence of the maximum principle for the Laplace equation:

If condition (7.3) holds for some β_0, it also holds for all $\beta > \beta_0$.

8. Numerical examples. In this section we consider the two examples of American call options from [8], which were also used in [16]. We compare the numerical result from using our new (approximated) discrete TBC to the solution using the discretized TBC (4.3) or (4.6) and use the explicit free boundary treatment from [16] described in §6. Since the method of [16] turned out to be superior to the projected SOR method with asymptotic boundary conditions we will compare our results only to the method of Han and Wu. In the sequel the dimension of time is year and dimension of value is US dollar.

8.1. Example 1. We consider an American call with an expiry of $T = 0.5$ years and a dividend yield $D_0 = 0.03$. The risk–free interest rate is $r = 0.03$, the volatility is $\sigma = 40\%$ p.a. and the exercise price is $E = \$100$. We choose a mesh ratio $\rho = 1$ and computed $N = 400$ time steps with different artificial boundary conditions at the left boundary $a = x_0 = -1.0$ which corresponds to an asset price $S = Ee^a \approx 36.79$. Fig. 8.1 shows the option values $V(S, 0)$ calculated with the exact discrete TBC (4.11). We recall the fact that all option values for $x < a$ can be calculated using (3.5) at the final time $\tau = \widetilde{T}$, i.e. at $t = 0$.

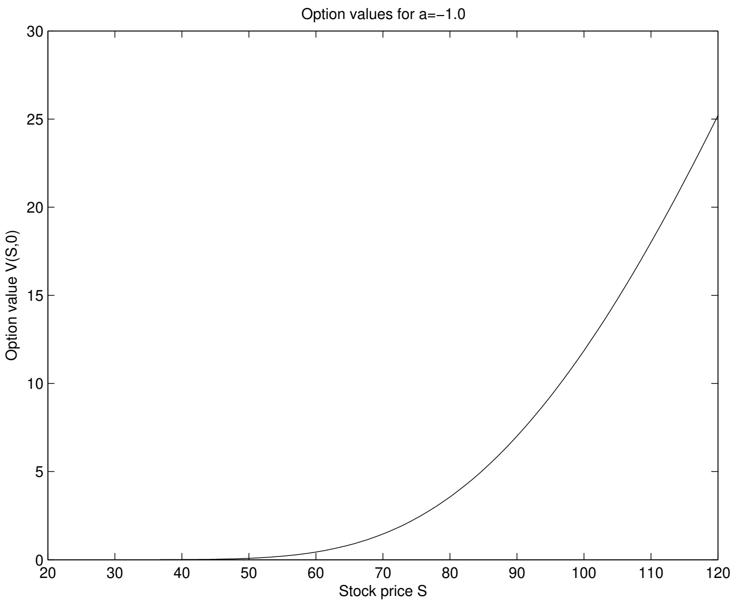

FIG. 8.1. *Option values V at time $t = 0$ (i.e. at $\tau = \widetilde{T}$).*

An upper bound of the free boundary $x_f(\tau)$ was calculated by (2.5) as $x_f^* = 1.5$. However the largest value of $x_f(\tau)$ is much smaller; it is about 0.62. The time evolution of the nondecreasing free boundary $x_f(\tau)$ is plotted in Fig. 8.2.

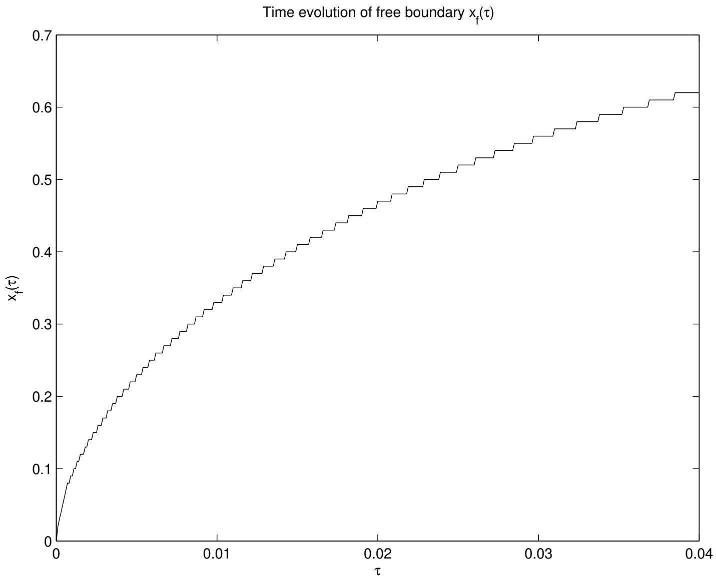

FIG. 8.2. *Time evolution of the free boundary $x_f(\tau)$ (the largest value of $x_f(\tau)$ is about 0.62)*

Next we want to investigate the stability of the scheme using the approximated discrete TBC (5.1) with $L = 20$ exponentials. Thus we have to check numerically the growth condition (7.3) needed for stability. It turned out that (7.3) is fulfilled for all $\beta \geq 1.42$. In Fig. 8.3 the real part of the transformed kernel $\hat{\tilde{\ell}}(z)$ of the approximated DTBC on the circle $z = \beta\, e^{i\varphi}$ with $\beta = -1.42$ is presented.

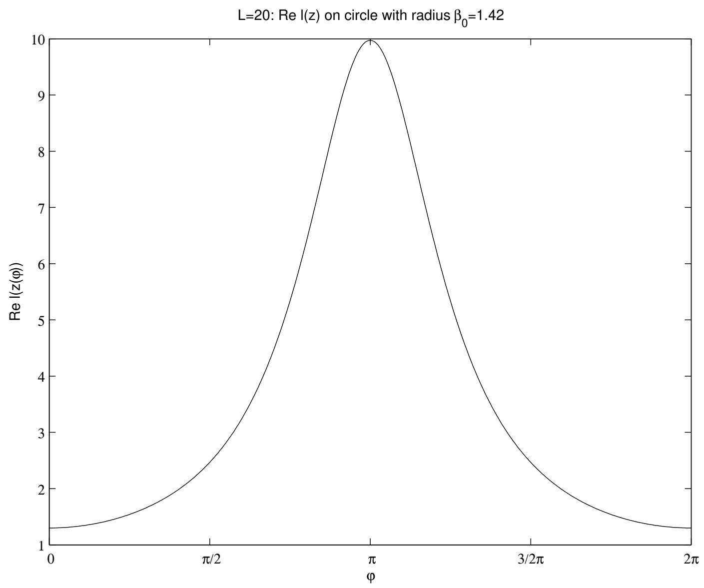

FIG. 8.3. *Growth condition* $\mathrm{Re}\, \hat{\tilde{\ell}}(z = \beta\, e^{i\varphi}) \geq 1$ *for the approximated discrete transparent boundary condition of* §5 *with* $L = 20$. *The stability condition* (7.3) *is satisfied for all* $\beta \geq 1.42$

Finally we want to compare the error when using the different artificial boundary conditions described previously. Since the discrete TBC (4.11) yields the exact numerical solution to the discrete problem (4.1) (up to round–off errors), we will take this solution as a reference solution v_{ref}. In order to make the induced errors more apparent we reduce the computational domain using $a = -0.2$ (which corresponds to an asset price $S = Ee^a \approx 81.87$). We plot in Fig. 8.4 the errors $\|v^{(n)} - v_{ref}^{(n)}\|_2^2$ measured in the discrete ℓ^2–norm (cf. (7.2)) on the computational interval.

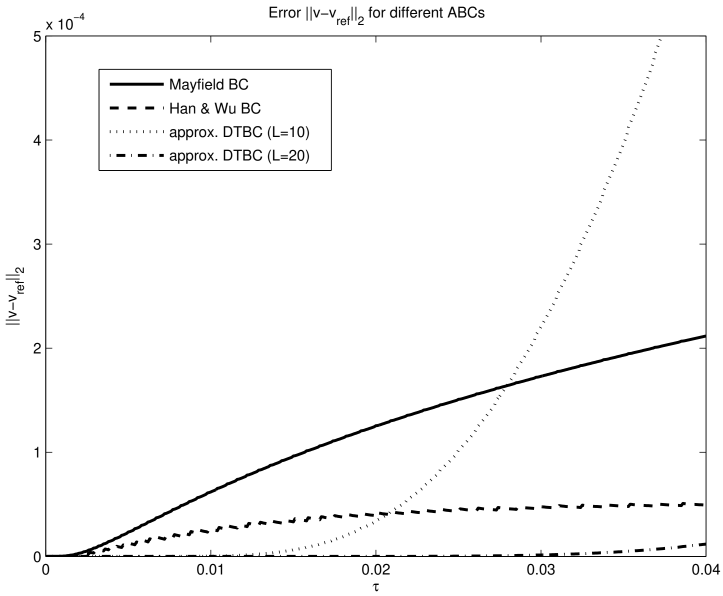

FIG. 8.4. *Error* $\|v^{(n)} - v_{ref}^{(n)}\|_2^2$ *for different artificial boundary conditions.*

The discretized TBC of Han & Wu (4.6) induced a smaller error than the discretized TBC of Mayfield (4.3) and the approximated discrete TBC (5.1) with $L = 10$. However, increasing the number of exponentials to $L = 20$ the approximated discrete TBC outperforms all other boundary conditions in this comparison.

In the second example we will consider a longer expiry time which is a more challenging task for the artificial boundary conditions.

8.2. Example 2. Now the parameters are expiry $T = 3$ years, risk–free interest rate $r = 0.03$, dividend yield $D_0 = 0.07$, volatility $\sigma = 40\%$ p.a., exercise price $E = \$100$, number of time steps $N = 400$ and mesh ratio $\rho = 1$. Fig. 8.5 shows the option values $V(S, 0)$ calculated with the exact discrete TBC (4.11) and $a = -1.0$.

Here the upper bound of the free boundary $x_f(\tau)$ was calculated to be $x_f^* = 0.8722$ and the largest value of $x_f(\tau)$ is about 0.71. Thus the estimate (2.5) is quite good in this example. In Fig. 8.6 the time evolution of the free boundary $x_f(\tau)$ is plotted.

As in the previous example we compare the error when using the different artificial boundary conditions and shrink the domain using $a = -0.2$ to make the differences in the approaches more visible. The resulting errors $\|v^{(n)} - v_{ref}^{(n)}\|_2^2$ in the discrete ℓ^2–norm are shown in Fig. 8.7. The results are comparable to the ones of Example 1 (cf. Fig. 8.4). The discretized TBC of Han & Wu (4.6) yielded more accurate results than the discretized TBC of Mayfield (4.3) and the approximated DTBC (5.1) with

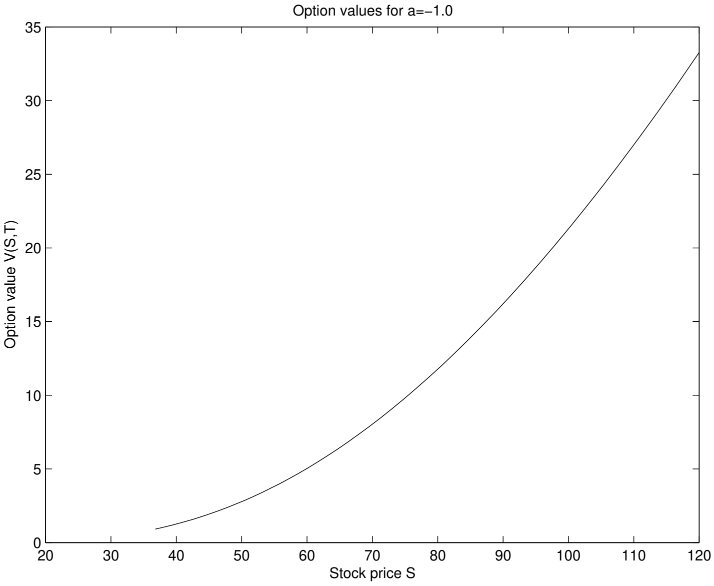

FIG. 8.5. *Option values V at time $t = 0$ (i.e. at $\tau = \widetilde{T}$).*

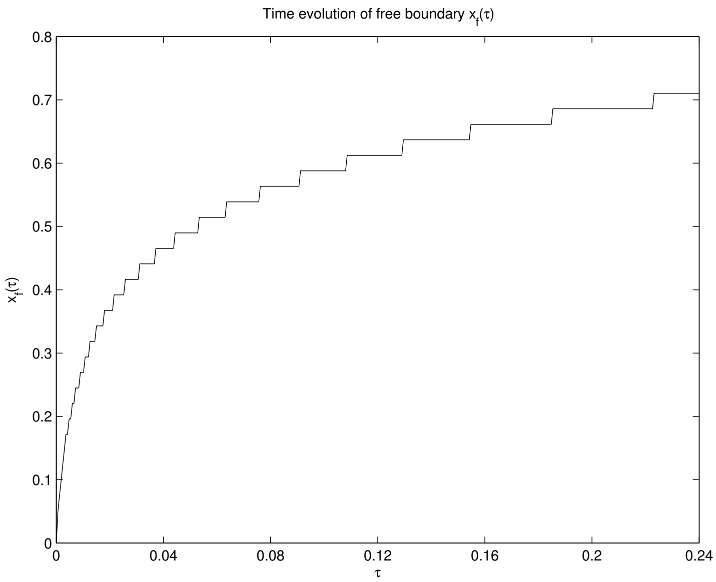

FIG. 8.6. *Time evolution of the free boundary $x_f(\tau)$ (the largest value of $x_f(\tau)$ is about 0.71)*

$L = 10$. But again the approximated DTBC with $L = 20$ exponentials turned out to be the best in this example. Note that the accuracy of the approximated DTBCs can be easily improved by increasing the parameter L in (5.1).

9. Conclusions and Outlook. In this paper we have derived an exact discrete artificial boundary condition for the Crank–Nicolson scheme for solving the Black–Scholes equation for the pricing of American options.

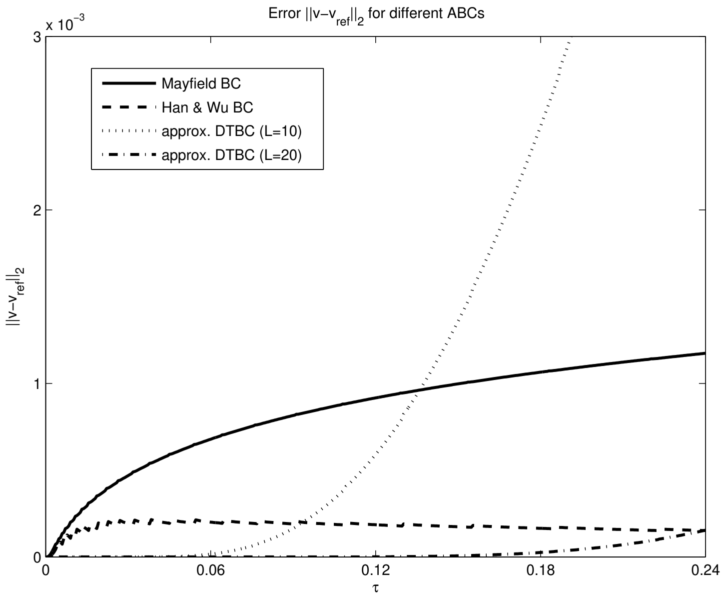

FIG. 8.7. *Error* $\|v^{(n)} - v_{ref}^{(n)}\|_2^2$ *for different artificial boundary conditions.*

To reduce the numerical effort we introduced a sum–of–exponentials approximation that leads to an artificial boundary condition that can be evaluated very efficiently. To ensure stability we proved a simple criteria and showed that it held for the exact artificial boundary condition. In the numerical examples all considered artificial boundary conditions yielded satisfactory results. However, the introduced approximated discrete TBC is faster (it does not increase the order of complexity of the interior scheme) and more accurate than existing discretized TBCs. Moreover its stability can be checked numerically in advance.

In this work we focused on standard options (known as *plain–vanilla options*) of American type. However, future work will deal with extensions: forward and future contracts, options on futures, general pay–off functions (e.g. 'cash–or–nothing call') with transaction costs and instalment options. Also, we will derive our DTBC for the *Crandall–Douglas Scheme* [23] which is fourth-order accurate in 'space' (i.e. asset price).

Appendix A. In the following table we list the coefficients $\{q_l, b_l\}$ of the sum–of–exponentials boundary condition with the convolution kernel (5.1) for the cases $L = 5$, and $L = 10$ with the "normalized" mesh ratio $\rho = 1$.

The coefficients b_l^*, q_l^* for another mesh ratio ρ_* can then be obtained from the explicit formulas in the Transformation rule 5.2. A Maple Code that was used to to calculate the coefficients q_l, b_l in the approximation (5.1) can be downloaded from the first author's homepage: www.math.tu-berlin.de/˜ehrhardt/.

	q_l	b_l
L=5	-4.1208652177	-.27811124956
	1.0967679400	-.18959940485e-1
	1.4922001539	-.10590997564
	2.9552027966	-.55958332115
	248.92225574	-3015.7838647
L=10	-9.9136756987937	-1.9875713184493
	-4.4195037755990	-.20293132298409
	-3.2680718769142	-.30208445829485e-1
	1.0274687817901	-.28888450814493e-2
	1.1170922091207	-.12593213109395e-1
	1.2954421237783	-.33173856847540e-1
	1.6304865463006	-.76395446779077e-1
	2.3151684017807	-.18317560643301
	4.1269461454773	-.58495741977923
	16.738352410466	-8.1688546950878

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