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Global regularity and probabilistic schemes for free boundary surfaces of multivariate American derivatives and their Greeks

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Abstract In a rather general setting of multivariate stochastic volatility market models we derive global iterative probabilistic schemes for computing the free boundary and its Greeks for a generic class of American derivative models using front-fixing methods. Establishment of convergence is closely linked to a proof of global regularity of the free boundary surface.

1. Introduction. The need of probabilistic representations of solutions of problems in finance is closely linked to the curse of dimensionality which enforces the application of Monte-Carlo methods especially for more intricate problems. The situation is especially challenging for nonlinear problems such as the free boundary problems related to pricing, hedging, and the optimal exercise strategies of American options. The present work establishes a stable iterative scheme which generates a sequence functions and their derivatives up to second order converging to the free boundary function (the image of which is the free boundary surface) and its derivatives for a standard class of American derivatives modelled in a quite general framework of diffusion type market models. Hence, it contributes to all these three financial problems. However, it is also a contribution to the theoretical question of regularity of the free boundary itself where we establish results which are neither covered by the general results of [5, 6] (cf. discusson below) nor by more special recent regularity results on American derivatives in [25, 28]. There are several methods in order to investigate regularity used in the literature. One is to differentiate equations in order to get equations for derivatives. Another is to find estimates for tangent paraboloids of the solutions (cf. [30, 31, 32]. Another is to find the solution in explicit form which is possible only in a very limited class of problems. In [6] the multivariate case of parabolic potential problem is investigated, i.e. the case of constant coefficients and with no assumption on the sign of the solution. The points of the free boundary are classified into regular and singular points by an energy and a density criterion and C^∞ regularity is proved around the regular points. Singular points are not considered. Hence, the regularity results of the present work which establishes overall regularity especially for the American basket Put option are not covered even in the case of the multivariate Black-Scholes model. However our results extend to a considerable class of models with variable coefficients. The only condition (beside regularity conditions on the coefficients) is a global graph condition which allows for a global transformation. Our method is based on the front fixing method. The term front-fixing refers to a nonlinear transformation to fix the free boundary and to solve the resulting non-linear problem. The transformation depends essentially on the data (in financial models on the final data).

The method of front fixing itself is discussed in several papers on univariate American options (cf. [23, 33]. In the univariate case these methods are less efficient than a moving boundary approach (cf. [22]). We shall investigate the American basket put option as the most prominent example treated in the literature. Regularity results for the American put option in the univariate case go back to [20] and [29] in the case of constant coefficients. In [11] the univariate case where coefficients depend on time and space. For a more recent contribution in the univariate case with variable coefficients cf. [3]. In the present work we obtain global regularity results for the American basket put. However, our method can be applied to the other most popular options (we shall provide a list below). In case of the Basket Put option we transform the free boundary problem to a nonlinear problem on a domain homeomorphic to a cube. We present the solution of the free boundary surface in terms of a nonlinear integral equations involving convolutions with transition densities of linear parabolic equations and linear Volterra equations. Analysis of this equations leads to regularity results which are simple (use of Banach fixed point theorem) and charming except that they involve some use of the Levy expansion of linear parabolic equations. Our main result here is the global regularity of the free boundary surface except for the final time T if a global graph condition is satisfied (which can be justified for a considerable class of models). The nonlinear integral equation is also the basis for our probabilistic scheme for computing the free boundary function, its time derivative and its spatial derivatives up to second order (Greeks). The only other Monte-Carlo method for computing the free boundary of a multivariate American Put option known to the author is [2, 21]. We break down the solution of this integral equation to an iteration of the solution of linear equations (essentially two parabolic equations and a linear Volterra integral equation). The corresponding convolutions with the transition density can be computed by WKB approximations (cf. [16, 17, 18]). Recent developments in the computations of Greeks with Monte-Carlo Methods (cf. [7, 13, 15]. Especially in [15] it is shown that WKB approximations can be a very efficient tool for the computation of Greeks for high-dimensional models. The convergence of the resulting iteration method is based on the regularity results for the free boundary.

The outline of the present article is as follows. In Section 2 we describe the general frame work of market models considered. We restrict ourselves to diffusion models (possibly with stochastic volatility). However extension especially to Levy models is possible. We formulate the free boundary problem to be solved. However the treatment of global operators in the context of free boundaries leads to additional involvements which will be consid-

ered elsewhere. In Section 3 we apply the front fixing method to the market models set up in the previous Section. We apply it especially for the American Put option (the most popular payoff function in the literature), but mention also other standard payoffs to which it may be applied. The free boundary problem set up in the previous section is globally transformed to a nonlinear problem on a hypercube. The free boundary function appears in the coefficients of this nonlinear parabolic function and is coupled to the boundary conditions. Especially the smooth fit condition of the original free boundary transforms is code into a mixed boundary condition on a hyperplane. The involved global graph condition which is formulated. Note that the possible failure of the smooth fit condition for general Levy models and beyond is one of the mentioned difficulties beyond market models with path-continuous models which make a detailed separated treatment of these models necessary. In Section 4 we derive a nonlinear integral equation which characterizes the free boundary and is based on the nonlinear initial boundary value problem characterizing the value function and established in the previous Section. In Section 5 a proof of the global existence and the regularity of the free boundary function is established. This is done via the nonlinear integral equation established in the previous Section. The integral equation is shown to determine a map of the Banach space of Hölder continuous functions with Hölder continuous derivatives up to the second order. Note that interior norms are used because the problem is not differentiable at maturity time and only C^1 on the boundary hyperplane where the mixed boundary condition is related to smooth fit condition of the original problem. The solution of the free boundary function is the fixed point of the nonlinear integral equation in the indicated Banach space. Global existence follows easily by standard theory of linear parabolic problems. In Section 6 an iteration scheme for the computation of the free boundary function and its Greeks is set up based on the regularity results of the previous Section and the nonlinear integral equation characterizing the free boundary function of Section 4. The description is distributed over four subsections. In the first subsection subproblems related to the nonlinear integral equation characterizing the free boundary function are identified. The second subsection recalls some recent results of the WKB expansion of the transition density (fundamental solution of linear parabolic equations). The third subsection describes the algorithm and the fourth subsection provides a convergence and qualitative error estimate analysis. A conclusion is given in Section 7 where we also indicate future research. Finally, in the appendix we add a technical proof needed in Section 5.

2. General framework. In this Section we shall set up the general framework and the technical conditions which are needed for the strong solutions of the systems of stochastic differential equations which model the underlyings (and possibly background processes) and the associated variational inequalities which determine the value of the American derivative written on that underlyings. Let O be an open domain in $\mathbb{R}^n$ and let $T \in (0, \infty)$ be the time horizon. We write $D = (0, T) \times O$ for the domain where O has to be specified case by case. For each starting point $(t, x) \in [0, T] \times O$, consider the following stochastic differential equation

$$\begin{aligned} & X_t^{t,x} = x \in O, \\ & dX_s^{t,x,k} = \mu_k(s, X_s^{t,x})ds + \textstyle\sum_{j=1}^m \sigma_{kj}(s, X_s^{t,x})dW_s^j, \end{aligned} \tag{2.1}$$

for continuous drift functions

$$\mu_k : [0, T] \times \mathbb{R}^n \to \mathbb{R}, \quad k = 1, \cdots, n, \tag{2.2}$$

and local volatility functions

$$\sigma_{ij} : [0, T] \times \mathbb{R}^n \to \mathbb{R} \quad i = 1, \cdots, n, \tag{2.3}$$

with an $\mathbb{R}^m$-valued Brownian motion $W = (W^j)_{j=1,\cdots,m}$ and where $X_s^{t,x} = (X_s^{t,x,k})_{k=1,\cdots,n}$. We assume that the functions μ_k and σ_{jk} are locally Lipschitz-continuous in x, uniformly in t, i.e. for each compact subset $K \subset \mathbb{R}^n$ there is a constant c (dependent on K) such that

$$|\mu_k(t, x) - \mu_k(t, y)| \leq c|x - y| \tag{2.4}$$

and

$$|\sigma_{ij}(t, x) - \sigma_{ij}(t, y)| \leq c|x - y| \tag{2.5}$$

for all $t \in [0, T]$ $x, y \in \Omega$. The latter assumption implies that (2.1) has a unique strong solution for any given filtered probability space $\left(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in[0,T]}, P\right)$ and Brownian motion W up to a possibly finite random explosion time. Therefore we add the assumption that

$$P\left(\sup_{s\in[t,T]} |X_s^{t,x}| < \infty\right) = 1. \tag{2.6}$$

Then theorem V. 38 of [26] implies that (2.1) has a strong solution. In this context we consider a stochastic volatility market model system with a

process S_t modeling the price of n assets and an d-dimensional background process Y driving the local volatility. Then for each starting point $(t,x) \in [0,T] \times \tilde{O} \subseteq \mathbb{R}^m_+ \times \mathbb{R}^d$ the stochastic differential equation

$$
\begin{aligned}
&(S_t^{t,x,y}, Y_t^{t,y}) = (x,y) \in \tilde{O}, \\
&\frac{dS_s^{t,x,k}}{S_s^{t,x,k}} = r(s, X_s^{t,x})ds + \textstyle\sum_{j=1}^n \sigma_{kj}(s, X_s^{t,x}, Y_s^{t,x}) dW_s^j, \\
&dY_s^{t,y,l} = \nu_l(s, Y_s^{t,x})ds + \textstyle\sum_{j=1}^p \beta_{lj}(s, Y_s^{t,x}) dW_s^j
\end{aligned}
\tag{2.7}
$$

has a unique strong solution, if the drift functions

$$
\begin{aligned}
&r : [0,T] \times \mathbb{R}^m \to \mathbb{R}, \\
&\nu_l : [0,T] \times \mathbb{R}^d \to \mathbb{R}, \quad l = 1, \cdots, d,
\end{aligned}
\tag{2.8}
$$

and the (volatility of) volatility functions

$$
\beta_{lj} : [0,T] \times \mathbb{R}^d \to \mathbb{R}, \quad l \in \{1, \cdots, p\}, \quad j \in \{1, \cdots, d\}
\tag{2.9}
$$

satisfy conditions of form (2.5) and (2.6) respectively.

Then the price $V(t,x,y)$ of an American option with payoff ϕ is given by

$$
V(t,x,y) := \sup_{\tau \in \mathrm{Stop}_{[t,T]}} E_Q \left[\exp\left(- \int_t^\tau r(s, S_t^{t,x,y}) \right) \phi\left(\tau, S_\tau^{t,x,y}\right) \right],
\tag{2.10}
$$

where $\mathrm{Stop}_{[t,T]}$ is the set of all $\mathcal{F}_t$ stopping times with value in $[t,T]$. The measure Q is some equivalent measure to be chosen if the market is incomplete and uniquely determined in a complete market. If the asset process S does not depend on a background process Y, then the market process is complete, especially $S_s^{t,x,y} \equiv S_s^{t,x}$. For simplicity of notation we deal with this situation in the following, noting that everything can be generalized to the more general incomplete market model (2.7) without problems (except the choice of the equivalent measure which is a problem of its own). Standard stochastic control theory can now be used to show that the value function $(t,x) \to V(t,x)$ satisfies the nonlinear Cauchy problem

$$
\begin{cases}
\max\left\{ \frac{\partial u}{\partial t} + Lu, \phi - u \right\} = 0, \text{ in } [0,T) \times \mathbb{R}^n \\
u(T,x) = \phi(T,x), \text{ in } \{T\} \times \mathbb{R}^n
\end{cases}
\tag{2.11}
$$

in the viscosity sense, where $v_{ij} = (\sigma\sigma^T)_{ij}$ and where

$$Lu \equiv \frac{1}{2}\sum_{ij} v_{ij} S_i S_j \frac{\partial^2 u}{\partial S_i \partial S_j} + r\left(\sum_i S_i \frac{\partial u}{\partial S_i} - u\right) \tag{2.12}$$

Global solutions for the latter type of equations in the viscosity sense were studied in [1] even in a far more general context. It is clear that (2.13) formally implies that

$$\begin{cases} \frac{\partial u}{\partial t} + Lu \leq 0, \\ \left(\frac{\partial u}{\partial t} + Lu\right)(\phi - u) = 0, \\ \phi - u \geq 0, \text{ in } [0,T) \times \mathbb{R}^n \text{ a.e.} \\ u(T,x) = \phi(T,x) \text{ on } \{T\} \times \mathbb{R}^n, \end{cases} \tag{2.13}$$

and where global solutions can be obtained under rather mild conditions by variational methods (cf. [12]). The equivalence of this system of variational inequalities with optimal stopping problems under relatively mild conditions have also be studied extensively (cf. [9]). The set points (t,x) where the value function u equals the obstacle ϕ is called the exercise region. The complement of the exercise region in the domain D is called the continuation reason. In [8] it is proved in a rather general context that the optimal stopping time is the first time where the value process hits the boundary of the exercise region. Therefore the free boundary surface (or the boundary of the exercise region) is crucial information in dealing with American Option. Especially in the context of hedging information concerning the Greeks near the free boundary is crucial. In the present article we set up a method to obtain the Greeks in a general class of multivariate models. Information of the value function in the continuation region and its Greeks are then a by-product of our method.

3. Frontfixing with special focus on American Basket Put options. We use a transformation involving the free boundary which is otherwise known as a frontfixing method. Our method works for a large class of options, e.g. for

- the minimum put with payoff $(K - \min\{S_1, S_2\})^+$,
- the spread with payoff $(K - (S_1 - S_2))^+$,
- the put on an index or index spreads $(K - \sum_{i=1}^n \alpha_i S_i)^+$,
- similar call options in standard models and other standard options.

Since suitable front-fixing depends on the pay-off we shall restrict the analysis to the most popular example the American Put on an index. It will be clear from the argument that the other options can be treated similarly. We start with the operator

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sum_{ij} v_{ij} S_i S_j \frac{\partial^2 u}{\partial S_i \partial S_j} + r\left(\sum_i S_i \frac{\partial u}{\partial S_i} - u\right), \tag{3.1}$$

where $v_{ij} = (\sigma\sigma^T)_{ij}$ and r may depend on time t and spatial variables S. Let $\mathcal{E}$ denote the exercise region and for each $t \in [0,T]$ let $\mathcal{E}_t$ denote the t-section of the exercise region, i.e. $\mathcal{E}_t := \{x|(t,x) \in \mathcal{E}\}$. In general beside basic standard assumptions on stochastic volatility models introduced in the previous Section we shall assume that

(GG) for each $t \in [0,T]$ $0 \in \mathcal{E}_t$ and that for a fixed "angle" at $S = (S_1, \cdots, S_n)$, i.e. at

$$\phi_S := \left(\frac{S_2}{\sum_{i=1}^n S_i}, \cdots, \frac{S_n}{\sum_{i=1}^n S_i}\right)$$

we have one intersection point of the section $\mathcal{E}_t$ and the intersection point of the ray through 0 which is determined by the angle ϕ_S.

Remark 3.1. We call (GG) the global graph condition. It is clear that this condition is satisfied for the multivariate Black-Scholes model and for a considerable class of stochastic volatility models. It is also satisfied by market models based on Levy processes. However, the latter type of models will be considered elsewhere.

Hence, the free boundary can be written in terms of the angles in form

$$(t, \phi_S) \to F(t, \phi_S). \tag{3.2}$$

We consider the transformation

$$\begin{aligned} &\psi : (0,T) \times \mathbb{R}^n_+ \to (0,T) \times [1,\infty) \times (0,1)^{n-1}, \\ &\psi(t, S_1, \cdots, S_n) = \left(\tau, \frac{\sum_{i=1}^n S_i}{F}, \frac{S_2}{\sum_{i=1}^n S_i}, \cdots, \frac{S_n}{\sum_{i=1}^n S_i}\right). \end{aligned} \tag{3.3}$$

Note that $\psi\left((0,T) \times \mathbb{R}^n_+\right)$ is homeomorph to the half space $H_{\geq 1} = \{x \in \mathbb{R}^n | x_1 \geq 1\}$. In the following the domain D is the interior of the image of ψ, i.e. $D := (0,T) \times (1,\infty) \times (0,1)^{n-1}$. We have

$$S_1 = x_1 F\left(1 - \sum_{j \geq 2} x_j\right), \; S_j = x_j x_1 F. \tag{3.4}$$

We get

$$
\begin{cases}
u_\tau = \frac{F_t}{F} x_1 \frac{\partial u}{\partial x_1} + \frac{1}{2} \sum_{ij} a_{ij}^F \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_j b_j^F \frac{\partial u}{\partial x_j} + r x_1 \frac{\partial u}{\partial x_1}, \\
(BC1) \quad u(0, \infty, x_2, \cdots, x_n) = 0 \text{ on } x_1 = \infty \\
(BC2) \quad u_{x_1}(t, 1, x_2, \cdots, x_n) - u(t, 1, x_2, \cdots, x_n) = -K \\
\qquad\qquad\qquad\qquad\qquad\qquad \text{on } x_1 = 1 \\
(BC3) \quad F(t, x_2, \cdots, x_n) = K - u(t, 1, x_2, \cdots, x_n) \\
(IC) \quad u(0, x) = \max\{K - x_1, 0\}
\end{cases} \tag{3.5}
$$

REMARK 3.2. We include (BC1) as an implicit boundary condition in order to indicate that (3.5) is equivalent to an initial-boundary value problem of the second type on a finite domain (just by suitable additional transformation with respect to the variable x_1).

The mixed condition $(BC2)$ follows from the smooth fit condition together with $(BC3)$.

REMARK 3.3. Note that in the context of market models based on Levy processes or, more generally, Feller processes the smooth fit condition does not hold in general and one has to be careful concerning generalization at this point. Especially one cannot expect that a condition of type $(BC3)$ holds in the pointwise sense if the smooth fit condition fails.

In order to determine the coefficients a_{ij}^F and b_i^F we compute first

$$
\begin{aligned}
F \frac{\partial x_j}{\partial S_i} &= \frac{\delta_{ij} - x_j}{x_1}, \\
F \frac{\partial x_j}{\partial S_1} &= 1 - \sum_{j \geq 2} (\delta_{ij} - x_j) \frac{F_j}{F}, \\
\frac{\partial}{\partial S_i} &= \sum_j \frac{\partial x_j}{\partial S_i} \frac{\partial}{\partial x_j}.
\end{aligned} \tag{3.6}
$$

We observe that

$$
\sum_i S_i \frac{\partial x_j}{\partial S_i} = \sum_i S_i \frac{\delta_{ij} - x_j}{x_1 F} = 0. \tag{3.7}
$$

It follows that

$$
\begin{aligned}
\textstyle\sum_i S_i \frac{\partial}{\partial S_i} &= \textstyle\sum_{ij} \frac{\partial x_j}{\partial S_i}\frac{\partial}{\partial S_i} \\
&= \textstyle\sum_i S_i \frac{\partial x_1}{\partial S_i}\frac{\partial}{\partial x_1} + \sum_{j\geq 2}\left(\sum_i S_i \frac{\partial x_1}{\partial S_i}\right)\frac{\partial}{\partial x_j} \\
&= \textstyle\sum_i S_i \frac{\partial x_1}{\partial S_i}\frac{\partial}{\partial x_1} \\
&= \textstyle\sum_i S_i \left(\frac{1}{F} - \sum_{j\geq 2}(\delta_{ij} - x_j)\frac{F_j}{F^2}\right)\frac{\partial}{\partial x_1} \\
&= x_1\frac{\partial}{\partial x_1} - \left(\textstyle\sum_i S_i\right)\left(\sum_{j\geq 2}\left(\frac{\partial x_j}{\partial S_i}\right)\frac{F_j}{F}x_1\right)\frac{\partial}{\partial x_1} \\
&= x_1\frac{\partial}{\partial x_1}.
\end{aligned}
\tag{3.8}
$$

Hence, we have

$$
r\left(\sum_i S_i \frac{\partial}{\partial S_i}\right) = r x_1 \frac{\partial}{\partial x_1}. \tag{3.9}
$$

It is clear that

$$
a_{ij}^F = \sum_{kl} v_{kl} S_k S_l \frac{\partial x_i}{\partial S_l}\frac{\partial x_l}{\partial S_k}, \tag{3.10}
$$

and that

$$
b_j^F = \sum_{kl} v_{kl} S_k S_l \frac{\partial^2 x_j}{\partial S_k \partial S_l}. \tag{3.11}
$$

In order to determine the latter coefficient function we compute

$$
\frac{\partial x_j}{\partial S_i} = \frac{1}{F}\frac{\delta_{ij} - x_j}{x_1}, j \geq 2 \tag{3.12}
$$

and

$$
\frac{\partial x_1}{\partial S_i} = \frac{1}{F}\left(1 - \sum_{j\geq 2}(\delta_{ij} - x_j)\frac{F_j}{F}\right). \tag{3.13}
$$

Next, for $j \geq 2$ we have

$$
\frac{\partial^2 x_j}{\partial S_i \partial S_k} = \sum_l \frac{\partial\left(\frac{\delta_{ij} - x_j}{F x_1}\right)}{\partial x_l}, \tag{3.14}
$$

and

$$\frac{\partial\left(\frac{\delta_{ij}-x_j}{Fx_1}\right)}{\partial x_l} = -\frac{\delta_{jl}}{x_1 F} + \frac{(x_j-\delta_{ij})(\delta_{1l}F + x_1 F_l(1-\delta_{1l})}{(x_1F)^2}. \tag{3.15}$$

Finally,

$$\frac{\partial^2 x_1}{\partial S_i \partial S_k} = \sum_l \frac{\partial}{\partial x_l}\left(\frac{1}{F} - \sum_{j\geq 2}(\delta_{ij}-x_j)\frac{F_j}{F^2}\right)\frac{\partial x_l}{\partial S_k}, \tag{3.16}$$

where

(3.17)

$$\begin{aligned}&\tfrac{\partial}{\partial x_l}\left(\tfrac{1}{F} - \textstyle\sum_{j\geq 2}(\delta_{ij}-x_j)\tfrac{F_j}{F^2}\right)\\ &= -\tfrac{F_l}{F^2}(1-\delta_{1l}) - \textstyle\sum_{j\geq 2}\tfrac{-\delta_{jl}F_j + (\delta_{ij}-x_j)F_{jl}(1-\delta_{1l}) - 2F_jF_l(1-\delta_{1l})(\delta_{ij}-x_j)}{F^3}.\end{aligned}$$

Here δ_{ij} is always the Kronecker Delta, F_j is short for $\frac{\partial F}{\partial x_j}$, F_{jl} is short for $\frac{\partial^2 F}{\partial x_j \partial x_l}$. Now we have determined the explicit form of (3.5). The next step is to construct a representation of the solution of (3.5) in terms of convolutions with the transition density, i.e the fundamental solution related to (3.5).

4. Derivation of a system of integral equations characterizing the free boundary. For a fixed free boundary function F we may consider (3.5) as a standard linear initial value boundary problem of the second type and of the form

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}\frac{\partial^2 u}{\partial x^i \partial x^j} + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x^i} = f, \text{ in } D\times(0,T] \tag{4.1}$$

$$u(0,x) = g(x) \text{ on } \overline{D} \tag{4.2}$$

$$\frac{\partial}{\partial \nu}u(t,x) + \alpha u(t,x) = h \text{ on } H\times(0,T], \tag{4.3}$$

where $H := \{x\in\mathbb{R}^n | x_1 = 1\}$ is part of the boundary of D (H is for 'hyperplane'). In the standard formulation of the initial value boundary problem ν denotes the inward normal and $a_{ij}, b_i, f, \alpha, h$ are functions which may depend on time t and the spatial variables x. In our case the derivative with respect to the inward normal reduces to the partial derivative $\frac{\partial}{\partial x_1}$, the function α is the constant function $\alpha \equiv -1$, h is the constant function $h = -K$, and $f \equiv 0$. Furthermore, the initial condition for the basket put is

just $g(x) = \max\{K - x_1, 0\}$ in the transformed coordinates. Hence equation (4.1) simplifies to

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}\frac{\partial^2 u}{\partial x^i \partial x^j} + \sum_{i=1}^{n} b_i \frac{\partial u}{\partial x^i} = 0, \text{ in } D \times (0,T] \tag{4.4}$$

$$u(0,x) = \max\{K - x_1, 0\} \text{ on } \overline{D} \tag{4.5}$$

$$\frac{\partial}{\partial x_1} u(t,x) - u(t,x) = -K \text{ on } H \times (0,T], \tag{4.6}$$

We represent the solution in terms of convolutions of the fundamental solution and an integral equation of Volterra type related to the mixed type boundary condition. First we define the fundmental solution $p \equiv p(t,x;\tau,y)$ for $t > \tau$ to solve for each (τ, y)

$$\frac{\partial u}{\partial t} + \frac{1}{2}\sum_{i,j=1}^{n} a_{ij}(t,x)\frac{\partial^2 u}{\partial x^i \partial x^j} + \sum_{i=1}^{n} b_i(x) \frac{\partial u}{\partial x^i} = 0, \text{ in } D \times (0,T] \tag{4.7}$$

$$u(0,x) = \delta_y(x) \text{ at } t = 0. \tag{4.8}$$

The general ansatz for (4.1)-(4.3) then is (recall that $\hat{x}_1 = (x_2, \cdots, x_n), \hat{y}_1 = (y_2, \cdots, y_n)$, and $dH_y = dy_2 dy_3 \cdots dy_n$)

$$\begin{aligned} u(t,x) = \quad & \int_0^t \int_H p(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi(\tau,1,\hat{y}_1) dH_y d\tau \\ & + \int_D p(t,x;0,y)g(y)dy - \int_0^t \int_D p(t,x;\tau,y)f(\tau,y)dyd\tau, \end{aligned} \tag{4.9}$$

where boundary condition $\frac{\partial}{\partial \nu} u(t,x) + \alpha(t,x)u(t,x) = h(t,x)$ then reduces to the Volterra type equation

$$\begin{aligned} \tfrac{1}{2}\phi(t,x) \quad & = \Gamma(t,x) + \\ & \int_0^t \int_H (\tfrac{\partial}{\partial x_1} p(t,1,\hat{x}_1,\tau,\hat{y}_1) + \alpha(t,1,\hat{x}_1)p(t,1,\hat{x}_1;\tau,1,\hat{y}_1)) \\ & \times \phi(\tau,1,\hat{y}_1) dH_y d\tau, \end{aligned} \tag{4.10}$$

with

$$\begin{aligned}\Gamma(t,x) = \quad & \textstyle\int_D \frac{\partial}{\partial x_1} p(t,x;0,y) g(y) dy \\ & + \textstyle\int_0^t \int_D \frac{\partial}{\partial x_1} p(t,x;\tau,y) f(\tau,y) dy d\tau \\ & + \alpha(t,x) \textstyle\int_D p(t,x;0,y) g(y) dy \\ & - \alpha(t,x) \textstyle\int_0^t \int_D p(t,x;\tau,y) f(\tau,y) dy d\tau \\ & - h(t,x).\end{aligned} \tag{4.11}$$

With $\alpha \equiv -1$, $h = -K$, and $f \equiv 0$, and $g(x) = \max\{K - x_1, 0\}$ this simplifies to

$$\begin{aligned}u(t,x) = \quad & \textstyle\int_0^t \int_H p(t,1,\hat{x}_1;\tau,1,\hat{y}_1) \phi(\tau,\hat{y}_1) dH_y d\tau \\ & + \textstyle\int_D p(t,x;0,y) \max\{K - y_1, 0\} dy,\end{aligned} \tag{4.12}$$

where

$$\begin{aligned}&\tfrac{1}{2}\phi(t,x) = \Gamma(t,x) + \\ &\textstyle\int_0^t \int_H (\frac{\partial}{\partial x_1} p(t,1,\hat{x}_1,\tau,\hat{y}_1) + p(t,1,\hat{x}_1;\tau,1,\hat{y}_1)) \phi(\tau,1,\hat{y}_1) dH_y d\tau,\end{aligned} \tag{4.13}$$

with

$$\begin{aligned}\Gamma(t,x) = \quad & \textstyle\int_D \frac{\partial}{\partial x_1} p(t,x;0,y) \max\{K - y_1, 0\} dy \\ & - \textstyle\int_D p(t,x;0,y) \max\{K - y_1, 0\} dy + K.\end{aligned} \tag{4.14}$$

We apply this to initial value boundary problem (3.5) in order to obtain a system of integral equations for the free boundary. First, from the boundary condition (BC3) in (3.5)

$$F(t,x_2,\cdots,x_n) = K - u(t,1,x_2,\cdots,x_n) \tag{4.15}$$

we get the integral equation

$$\begin{aligned}F(t,x_2,\cdots,x_n) = \quad & K - u(t,1,\hat{x}_1) = \\ & K - \textstyle\int_0^t \int_H p(t,1,\hat{x}_1;\tau,1,\hat{y}_1) \phi(\tau,1,\hat{y}_1) dH_y d\tau \\ + \quad & \textstyle\int_D p(t,x;0,y) \max\{K - y_1, 0\} dy.\end{aligned} \tag{4.16}$$

Note that the function ϕ which is itself solution of a linear integral equation and can itself be represented in terms of the fundamental solution. Define

$$\frac{1}{2}Z_F^1(t,x;\tau,y) = \frac{\partial}{\partial x_1}p_F(t,x;0,y) - p_F(t,x;0,y), \tag{4.17}$$

and for $r \geq 1$ define

$$Z_F^{r+1}(t,x,\tau,y) = \int_0^t \int_H Z_F^r(t,x,\sigma,1,\hat{z}_1)Z_F^r(\sigma,\hat{z}_1,\tau,y)dH_y d\sigma \tag{4.18}$$

Then

$$\frac{1}{2}\phi(t,x) = \Gamma(t,x) + \sum_{r=1}^{\infty}\int_0^t \int_H Z_F^r(t,x,\tau,1,\hat{y}_1)dH_y d\tau \tag{4.19}$$

We summarize

THEOREM 4.1. *Assume that (GG) and the assumptions of the general framework hold. Then the free boundary surface function F of the multivariate American basket put option (with weights normalized to 1 w.l.o.g.) in the transformed coordinates*

$$\begin{aligned} &\psi : (0,T)\times\mathbb{R}_+^n \to (0,T)\times[1,\infty)\times(0,1)^{n-1} \\ &\psi(t,S_1,\cdots,S_n) = \left(\tau, \frac{\sum_{i=1}^n S_i}{F}, \frac{S_2}{\sum_{i=1}^n S_i}, \cdots, \frac{S_n}{\sum_{i=1}^n S_i}\right) \end{aligned} \tag{4.20}$$

is solution of the integral equation

$$\begin{aligned} F(t,x_2,\cdots,x_n) = K - u(t,1,\hat{x}_1) = \\ K - \textstyle\int_0^t \int_H p_F(t,1,\hat{x}_1;\tau,y)\phi(\tau,y)dH_y d\tau \\ + \textstyle\int_D p_F(t,1,\hat{x}_1;0,y)\,(K-y_1)^+\,dy, \end{aligned} \tag{4.21}$$

where

$$\frac{1}{2}\phi(t,x) = \Gamma(t,x) + \sum_{r=1}^{\infty}\int_0^t \int_S Z_F^r(t,x,\tau,1,\hat{y}_1)dH_y d\tau \tag{4.22}$$

with

$$\frac{1}{2}Z_F^1(t,x;\tau,y) = \frac{\partial}{\partial x_1}p_F(t,x;0,y) - p_F(t,x;0,y), \tag{4.23}$$

$$Z_F^{r+1}(t,x,\tau,y) = \int_0^t \int_H Z_F^r(t,x,\sigma,z) Z_F^r(\sigma,z,\tau,1,\hat{y}_1) dH_y d\sigma, \tag{4.24}$$

for $r \geq 1$, *and* p_F *is the fundamental solution of*

$$u_\tau = \frac{F_t}{F} x_1 \frac{\partial u}{\partial x_1} + \frac{1}{2} \sum_{ij} a_{ij}^F \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_j b_j^F \frac{\partial u}{\partial x_j} + r x_1 \frac{\partial u}{\partial x_1}. \tag{4.25}$$

REMARK 4.2. Note that the fundamental solution of (4.25) can be given in the form of a Levy expansion, i.e.

$$p^F(t,x,\tau,y) = Z^F(t,x,\tau,y) + \int_\tau^t \int_D Z^F(t,x,s,z) \Phi^F(s,z,\tau,y) dz ds \tag{4.26}$$

where

$$\Phi^F(t,x,\tau,y) = \sum_{n=1}^{\infty} (L^F Z)_n(t,x,\tau,y) \tag{4.27}$$

(4.28)

$$(L^F Z)_1(t,x,\tau,y) = L^F Z^F(t,x,\tau,y),$$

$$(L^F Z)_{n+1}(t,x,\tau,y) = \textstyle\int_\tau^t \int_D L^F Z^F(t,x,s,z)(L^F Z)_n(s,z,\tau,y) dz ds,$$

where $Z^F(t,x,\tau,y) = \frac{1}{\sqrt{2\pi(t-\tau)}^n} \sqrt{\det A_F^{-1}(\tau,y)} \exp\left(- \frac{a_F^{ij}(\tau,y)(x_i - y_i)(x_j - y_j)}{2(t-\tau)} \right)$

with $\det A_F^{-1}(\tau,y) = a_F^{ij}(\tau,y)$ being the inverse of $(a_{ij}^F(\tau,y))$. The Levy expansion is not an efficient tool in order to compute the fundamental solution, but we shall use it for proving existence and uniqueness of the free boundary function below.

5. Global existence and uniqueness of solutions. From the relation

$$F(t,\hat{x}_1) = K - u(t,1,\hat{x}_1) \tag{5.1}$$

(recall that $(x_2, \cdots, x_n) = \hat{x}_1$) it is clear that uniqueness of u implies uniqueness of F and vice versa. Moreover, the initial value (free)-boundary problem (3.5) can be written as a nonlinear initial value boundary problem as in (5.2) below. Indeed, let

$$u^1(t,\hat{x}_1) = u(t,1,\hat{x}_1)$$

and let us denote by $a_{ij}^{u^1}$ and $b_j^{u^1}$ the coefficient functions obtained from a_{ij}^F and b_j^F substituting F by $K-u^1$ and the derivatives of F by the derivatives of $-u^1$. Then we have

$$
\begin{cases}
u_\tau = -\frac{u_t^1}{u^1} x_1 \frac{\partial u}{\partial x_1} + \frac{1}{2}\sum_{ij} a_{ij}^{u^1} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_j b_j^{u^1} \frac{\partial u}{\partial x_j} + r x_1 \frac{\partial u}{\partial x_1}, \\
(BC1)\quad u(t,\infty,x_2,\cdots,x_n) = 0 \text{ on } x_1 = \infty, \\
(BC2)\quad u_{x_1}(t,1,x_2,\cdots,x_n) - u(t,1,x_2,\cdots,x_n) = -K, \quad \text{if } x_1 = 1 \\
(IC)\quad u(0,x) = \max\{K - x_1, 0\}.
\end{cases} \tag{5.2}
$$

It is clear from our representation that once regularity of the free boundary surface is guaranteed, global existence of the solution can be obtained from (5.2). We shall prove regularity of the free boundary function by using the integral equation in theorem 4.1. The idea is to look at this integral equation as a map of a suitable Banach space where the free boundary function is obtained as a fixed point. In order to state the theorem we recall the definition of Banach spaces related to Schauder estimates. Schauder boundary estimates turn out to be appropriate since the problem in (3.5) is equivalent to a problem on a bounded domain with Dirichlet conditions on a transformed hyperplane H_∞. Therefore we denote the boundary of (3.5) by

$$
\partial D = H_1 \cup H_\infty \cup I \cup F \tag{5.3}
$$

and, for convenience, we define

$$
S := H_1 \cup H_\infty \tag{5.4}
$$

with

$$
\begin{aligned}
H_1 := H &= \{(t,x) \in (0,T) \times \mathbb{R}^n | x_1 = 1\}, \\
H_\infty &:= \{(t,x) \in (0,T) \times \mathbb{R}^n | x_1 = \infty\}, \text{and} \\
I &= \{(t,x) \in [0,T] \times \mathbb{R}^n | x_1 \geq 1 \text{ and } t = 0\} \\
F &= \{(t,x) \in [0,T] \times \mathbb{R}^n | x_1 \geq 1 \text{ and } t = T\}.
\end{aligned} \tag{5.5}
$$

We assume that (3.5) has been transformed to a finite domain (a suitable additional transformation with respect to the variable x_1 s easily constructed).

We therefore may assume in the following that $D \subset \mathbb{R}^{n+1}$ is a bounded domain. Abbreviating $\frac{\partial}{\partial x_i} =: D_{x_i}$, $\frac{\partial^2}{\partial x_i \partial x_j} =: D_{x_i x_j}$, $\frac{\partial}{\partial t} =: D_t$.

For any points $P \in S$ and $Q \in D$ define the distance from Q to S by

$$d_Q := \inf_{P \in S} d(P, Q), \tag{5.6}$$

where $d(P, Q)$ denotes the Euclidean distance between $P = (t, x)$ and $Q = (s, y)$, i.e.

$$d(P, Q) = \sqrt{|x - y|^2 + |t - s|^2}. \tag{5.7}$$

Furthermore, for any two points $P, Q \in D$, integers $m \geq 1$ and any function $v : D \to \mathbb{R}$ let $d_{PQ} = \min\{d_p, d_Q\}$ and define

$$\delta_\alpha^D(d^m f) := \mathrm{lub}_{P,Q \in D} d_{PQ}^{m+\alpha} \frac{|v(P) - v(Q)|}{d(P, Q)^\alpha}, \tag{5.8}$$

and

$$|v|_\alpha^D = \sup_{(t,x) \in D} |v(t, x)| + \delta_\alpha^D(v) \tag{5.9}$$

Let

$$|v|_{2+\alpha}^D = |v|_\alpha^D + \sum_{i=1}^n |dD_{x_i} v|_\alpha^D + \sum_{ij=1}^n |d^2 D_{x_i x_j} v|_\alpha^D + |d^2 D_t v|_\alpha^D, \tag{5.10}$$

and define

$$C_{2+\alpha}(D) := \left\{ f : D \to \mathbb{R} || f|_{2+\alpha}^D < \infty \right\} \tag{5.11}$$

Recall that

PROPOSITION 5.1. *If D is bounded, then $C_{2+\alpha}(D)$ is a Banach space.*

Next we recall some classical results on a priori estimates by Schauder. Consider the first initial-boundary value problem

$$\begin{cases} \frac{\partial w}{\partial t} - \frac{1}{2} \sum_{ij} a_{ij}(t, x) \frac{\partial^2 w}{\partial x_i \partial x_j} - \sum_i b_i(t, x) \frac{\partial w}{\partial x_i} + c(t, x) w = f(t, x) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{in } D \cup F, \\ \\ w(t, x) = h(t, x) \text{ on } I \cup H, \end{cases} \tag{5.12}$$

and assume that the following assumptions are satisfied:

(A) the coefficients $(t,x) \to a_{ij}(t,x)$ satisfy an ellipticity condition, i.e. there exists a constant $C > 0$ such that for any $(t,x) \in D$

$$\sum_{ij} a_{ij}(t,x)\xi_i\xi_j \geq c|\xi|^2. \tag{5.13}$$

(B) The coefficient functions $(t,x) \to a_{ij}(t,x)$ and $(t,x) \to b_i(t,x)$ and $(t,x) \to c(t,x)$ are locally Hölder continuous (exponent α), i.e. there exists a constant $C > 0$ such that

$$|a_{ij}|_\alpha \leq C, |db_i|_\alpha \leq C, |d^2c|_\alpha \leq C \tag{5.14}$$

(C) the function f is locally Hölder continuous (exponent α), i.e. there exists a constant $C > 0$ such that

$$|d^2 f|_\alpha \leq C \tag{5.15}$$

DEFINITION 5.2. We say that S has the outside strong sphere property if for every $Q = (t,x) \in S$ there exists a ball B with center (t_m, x_m) such that $B \cap \overline{D} = Q$ and $|x - x_m| \geq \lambda(Q) > 0$ for all $(t,x) \in \overline{D}$ and $|t - t_m| \leq \epsilon$.

We observe

PROPOSITION 5.3. *The boundary surface H has the outside strong sphere property.*

Proof. Trivial.
Now a classical result on Schauder estimates states that

THEOREM 5.4. *Assume that (A), (B), and (C) hold and assume that S has the outside strong sphere property. Then for any continuous function h on $I \cup H$ there exists a unique solution of the (5.12), and $u \in C_{2+\alpha}(D)$.*

Now we can establish the main result.

THEOREM 5.5. *Assume that the assumption of the general framework, the assumptions (A), and (B) of the present section hold for the domain D, and the global graph condition (GG) holds. Then free boundary function $F :]0,T[\times]0,1[^{n-1} \to \mathbb{R}$ in (3.5) is in $C_{2+\alpha}(D)$.*

Proof. The main observation here is that we can use a priori estimates of the first initial-boundary value problem to study the regularity of a class of

linear second initial-boundary value problems. We first show that there is a function

$$
\begin{aligned}
& G : C_{2+\alpha}(D) \to C_{2+\alpha}(D) \\
& G(v)(t,x) = K - \int_0^t \int_H p_v(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_v(\tau,1,\hat{y}_1)dH_y d\tau \\
& \qquad\qquad + \int_D p_v(t,1,\hat{x}_1;0,y)\,(K-y_1)^+\,dy,
\end{aligned} \tag{5.16}
$$

i.e. we show that G as specified in (5.16) is indeed a function from $C_{2+\alpha}(D)$ to $C_{2+\alpha}(D)$. Note that the classical theory of the fundamental solution (Levy expansion) immediately implies that $(t,x) \to G(v)(t,x)$ is continuously differentiable with respect to time and twice continuously differentiable with respect to the spacial variables for $v \in C_{2+\alpha}(D)$. However, both integrals in (5.16) have an interpretation as an inititial-boundary problem of type (5.12) (note the implicit data on the boundary) and application of theorem 5.4. leads to the conclusion that G is indeed a map of $C_{2+\alpha}(D)$.

LEMMA 5.6. *For all $t \in [0,T]$, $x \in D$ and $w_1, w_2 \in C_{2+\alpha}(D)$ there is a constant $L < \infty$ such that*

$$
|G(w_1) - G(w_2)|^D_{2,\alpha} \leq Lt|w_1 - w_2|^D_{2,\alpha}. \tag{5.17}
$$

Proof. The proof is not difficult but technically cumbersome. We indicate the basic idea. The proof is based on the Levy expansion of the fundamental solution. For fixed $w_i, i \in \{1,2\}$ consider the Levy expansions (cf. remark 4.2.) of the fundamental solution

$$
p^{w_i}(t,x,\tau,y) = Z^{w_i}(t,x,\tau,y) + \int_\tau^t \int_D Z^F(t,x,s,z)\Phi^{w_i}(s,z,\tau,y)dzds \tag{5.18}
$$

where

$$
\Phi^{w_i}(t,x,\tau,y) = \lim_{m\uparrow\infty} \Phi^{w_i}_m(t,x,\tau,y) := \lim_{m\uparrow\infty} \sum_{n=1}^{m} (L^F Z)_n(t,x,\tau,y), \tag{5.19}
$$

and its derivatives up to second order. Note that the second spatial derivatives have the form

$$
\begin{aligned}
p^{w_i}(t,x,\tau,y) = \; & \tfrac{\partial^2}{\partial x_i \partial x_j} Z^{w_i}(t,x,\tau,y) \\
& + \int_\tau^t \int_D \tfrac{\partial^2}{\partial x_i \partial x_j} Z^F(t,x,s,z)\Phi^{w_i}(s,z,\tau,y)dzds,
\end{aligned} \tag{5.20}
$$

the first time derivative has the form

$$
\begin{aligned}
p^{w_i}(t,x,\tau,y) = \quad & \tfrac{\partial}{\partial t} Z^{w_i}(t,x,\tau,y) - \Phi^{w_i}(t,x,z,\tau,y) \\
& + \int_\tau^t \int_D \tfrac{\partial}{\partial t} Z^F(t,x,s,z) \Phi^{w_i}(s,z,\tau,y) dz ds,
\end{aligned} \tag{5.21}
$$

and the first order spatial derivatives are of the form

$$
\begin{aligned}
p^{w_i}(t,x,\tau,y) = \quad & \tfrac{\partial}{\partial x_i} Z^{w_i}(t,x,\tau,y) \\
& + \int_\tau^t \int_D \tfrac{\partial^2}{\partial x_i} Z^F(t,x,s,z) \Phi^{w_i}(s,z,\tau,y) dz ds.
\end{aligned} \tag{5.22}
$$

Inserting these expressions into $|G(w_1) - G(w_2)|^D_{2,\alpha}$ and using triangle inequalities and induction over m leads to the desired result.□

We conclude that the function $G : C_{2+\alpha}(D) \to C_{2+\alpha}(D)$ is a contraction and its unique fixed point, and the back transformation with respect to x_1 of this fixed point is the free boundary function F, which is hence in $C_{2+\alpha}(D)$.

6. Iterative schemes for the free boundary surface and the Greeks. The contraction map G in the regularity proof above leads to various versions of iterative schemes for the free boundary surface F, its time derivative and its spacial derivatives up to second order. We describe an algorithmic scheme which has several possible realizations (probabilistic and PDE-schemes) of its subproblems. We shall describe the probabilistic scheme in more detail. PDE-schemes and issues of implementation will be considered elsewhere.

6.1. *Splitting scheme (splitting the mixed boundary problem at each iteration step).* In the proof of theorem (5.5) we observed that the free boundary function F is a fixed point of the intergal equation

$$
\begin{aligned}
F(t,\hat{x}_1) = K & - \int_0^t \int_H p_F(t,1,\hat{x}_1;\tau,1,\hat{y}_1) \phi_F(\tau,1,\hat{y}_1) dH_y d\tau \\
& + \int_D p_F(t,x;0,y) \max\{K - y_1, 0\}\, dy.
\end{aligned} \tag{6.1}
$$

along with a linear integral equation for ϕ_F. Now given a function $F \in C_{2+\alpha}(D)$ we may first solve for the linear integral equation for ϕ_F. This is a Volterra integral equation well-studied in the literature numerically (cf. [27] for a probabilistic treatment). Next we analyze (6.1). First, the term

$$
\int_D p_F(t,x;0,y) \max\{K - y_1, 0\}\, dy \tag{6.2}
$$

can be interpreted to be the solution of

$$\text{(6.3)}\qquad \begin{cases} u_\tau = \frac{F_t}{F} x_1 \frac{\partial u}{\partial x_1} + \frac{1}{2}\sum_{ij} a^F_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_j b^F_j \frac{\partial u}{\partial x_j} + r x_1 \frac{\partial u}{\partial x_1}, \\ (IC)\quad u(0,x) = \max\{K - x_1, 0\} \end{cases}$$

on D with natural boundary conditions on H. The interpretation of

$$\text{(6.4)}\qquad \int_0^t \int_H p_F(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_F(\tau,1,\hat{y}_1) dH_y d\tau$$

as a solution of a Cauchy problem with initial condition equal to zero and a source related to ϕ_F of reduced dimension $n-1$ is more theoretical in the sense that a statement of the related lower dimensional Cauchy problem is in general only possible if the solution u is known. This is a first reason why an efficient computation of the transition density (fundamental solution) is desirable, and it also indicates that our algorithm is intrinsically probabilistic to some extent in the sense that it cannot be completely realized without referring to the transition density. A second reason is the following. If we know the fundamental solution p_F in (6.24) and in (6.3) (for fixed F), then we can obtain the expressions $p_{F,t}$, $p_{F,x_i}, i \in \{2,\cdots,n\}$, and $p_{F,x_i x_j}, i,j \in \{2,\cdots,n\}$ for the next iteration step $n+1$ by differentiation under the integral, i.e given the approximation of the free boundary surface of the n-th iteration step F^n and its derivatives occurring in p_{F_n} we get the approximation of the free boundary surface of the $n+1$-th iteration step F^{n+1} and its derivatives F^{n+1}_t, $F^{n+1}_{x_i}, i \in \{2,\cdots,n\}$, and $F^{n+1}_{x_i x_j}, i,j \in \{2,\cdots,n\}$ via

$$\text{(6.5)}\qquad \begin{aligned} \frac{\partial}{\partial t} F^{n+1}(t,\hat{x}_1) &= -\frac{\partial}{\partial t}\int_0^t \int_H p_{F^n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_{F^n}(\tau,1,\hat{y}_1) dH_y d\tau \\ &\quad + \int_D \frac{\partial}{\partial t} p_{F^n}(t,x;0,y)\max\{K-y_1,0\}\, dy \\ \frac{\partial}{\partial x_i} F^{n+1}(t,\hat{x}_1) &= -\int_0^t \int_H \frac{\partial}{\partial t} p_{F^n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_{F^n}(\tau,1,\hat{y}_1) dH_y d\tau \\ &\quad + \int_D \frac{\partial}{\partial t} p_{F^n}(t,x;0,y)\max\{K-y_1,0\}\, dy \\ \frac{\partial^2}{\partial x_i \partial x_j} F^{n+1}(t,\hat{x}_1) &= -\int_0^t \int_H \frac{\partial^2}{\partial x_i \partial x_j} p_{F^n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\times \\ &\quad \phi_{F^n}(\tau,1,\hat{y}_1) dH_y d\tau + \int_D \frac{\partial^2}{\partial x_i \partial x_j} p_{F^n}(t,x;0,y)\max\{K-y_1,0\}\, dy \end{aligned}$$

Note that

$$\begin{aligned}\frac{\partial}{\partial t}F^{n+1}(t,\hat{x}_1) &= -\int_0^t\int_H \frac{\partial}{\partial t}p_{F^n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_{F^n}(\tau,1,\hat{y}_1)dH_y d\tau \\ &+ \int_H p_{F^n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_{F^n}(t,1,\hat{y}_1)dH_y \\ &+ \int_D \frac{\partial}{\partial t}p_{F^n}(t,x;0,y)\max\{K-y_1,0\}\,dy,\end{aligned} \tag{6.6}$$

giving a formula for $\frac{\partial}{\partial t}F^{n+1}$ in terms of the transition density p_{F^n}. As we observed in [15], approximating derivatives of value functions by derivatives of analytical approximations of transition densities in convolution representations of the value function is numerically efficient and allows for error estimates in strong norms by using a priori estimates of Safonov type (cf. [19]), and applying them to analytical representations of the transition density and its approximations (cf. [15]). The WKB-expansion of the transition density is such an analytical representation.

6.2. *Use of WKB-expansions of the fundamental solution at each iteration step.* We review some recent research on the fundamental solution (transition density), i.e. some results concerning WKB-expansions of parabolic equations (cf. [15, 17], for more details). The solution $(t,x,s,y)\to p(t,x,s,y)$ of the family of parabolic equations

$$\begin{aligned}&\tfrac{\partial u}{\partial t} - \tfrac{1}{2}\textstyle\sum_{i,j} a_{ij}\frac{\partial^2 u}{\partial x_i\partial x_j} - \sum_i b_i\frac{\partial u}{\partial x_i} = 0 \\ &p(0,x,0,y) = \delta(x-y),\end{aligned} \tag{6.7}$$

on a domain D, parameterized by $y\in\mathbb{R}^n$, and where δ denotes the Dirac delta distribution and the diffusion coefficients a_{ij} and the first order coefficients b_i in (6.7) may depend on time t and the spatial variable x. Without loss of generality and for simplicity of notation we consider the case where the coefficients depend on the spatial coordinates. Note that the time coordinate in the coefficients can be treated as an extra spatial coordinate and the resulting degenerate parabolic equation belongs to a class of so-called projective parabolic equations which are subject to all the following results (cf. [18]), In the following let $\delta t := t-s$, and let the functions

$$(x,y)\to d(x,y)\geq 0,\quad (x,y)\to c_k(x,y),\ k\geq 0,$$

be defined on $[0,T]\times\mathbb{R}^n\times[0,T]\times\mathbb{R}^n$. Then a set of (simplified) conditions sufficient for pointwise valid WKB-representations of the form

$$p(t,x,s,y) = \frac{1}{\sqrt{2\pi\delta t}^n}\exp\left(-\frac{d^2(x,y)}{2\delta t} + \sum_{k=0}^{\infty} c_k(x,y)\delta t^k\right), \tag{6.8}$$

is given by

(WKB1) The operator L is uniformly elliptic in $\mathbb{R}^n$, i.e. the matrix norm of $(a_{ij}(t,x))$ is bounded from below by $\lambda > 0$ and from above by $\Lambda > \lambda$, uniformly in x,

(WKB2) the smooth functions $(t,x) \to a_{ij}(t,x)$ and $(t,x) \to b_i(t,x)$ and all their derivatives are bounded.

For more subtle (and partially weaker conditions) we refer to [17]. If we add the uniform boundedness condition

(WKB3) there exists a constant c such that for each multiindex $\alpha \in \mathbb{N}^n$, and for all $1 \leq i,j,k \leq n$,

$$\left|\frac{\partial^\alpha a_{jk}}{\partial x^\alpha}(x)\right|, \left|\frac{\partial^\alpha b_i}{\partial x^\alpha}(x)\right| \leq c \exp\left(c|x|^2\right), \tag{6.9}$$

then the Taylor expansions of the functions d and c_k around $y \in \mathbb{R}^n$ are equal to d and $c_k, k \geq 0$ globally, i.e. we have the power series representations

$$\begin{aligned} d^2(x,y) &= \textstyle\sum_\alpha d_\alpha(y)\delta x^\alpha \\ c_k(x,y) &= \textstyle\sum_\alpha c_{k,\alpha}(y)\delta x^\alpha, \qquad k \geq 0, \end{aligned} \tag{6.10}$$

where $\delta x := x - y$. Note that (C) is implied by the stronger condition that all derivatives in (6.9) have a uniform bound. Summing up we have the following theorem:

THEOREM 6.1. *If the hypotheses (A),(B) are satisfied, then the fundamental solution p has the representation*

$$p(\delta t, x, y) = \frac{1}{\sqrt{2\pi\delta t}^n} \exp\left(-\frac{d^2(x,y)}{2\delta t} + \sum_{k\geq 0} c_k(x,y)\delta t^k\right), \tag{6.11}$$

where d and c_k are smooth functions, which are unique global solutions of the first order differential equations (6.12),(6.13), and (6.15) below. Especially,

$$(\delta t, x, y) \to \delta t \ln p(\delta t, x, y) = -\frac{n}{2}\delta t \ln(2\pi\delta t) - \frac{d^2}{2} + \sum_{k\geq 0} c_k(x,y)\delta t^{k+1}$$

is a smooth function which converges to $-\frac{d^2}{2}$ as $\delta t \searrow 0$, where d is the Riemannian distance induced by the line element $ds^2 = \sum_{ij} a_{ij}^{-1} dx_i dx_j$, where with a slight abuse of notation (a_{ij}^{-1}) denotes the matrix inverse of (a_{ij}). If the hypotheses (A),(B) and (C) are satisfied, then in addition the functions d, $c_k, k \geq 0$ equal their Taylor expansion around y globally.

The recursion formulas for d and c_k, $k \geq 0$ are obtained by plugging the ansatz (6.8) into the parabolic equation (6.7), and ordering terms with respect to the monoms $\delta t^i = (T-t)^i$ for $i \geq -2$. By collecting terms of order δt^{-2} we obtain

$$d^2 = \frac{1}{4} \sum_{ij} d^2_{x_i} a_{ij} d^2_{x_j}, \tag{6.12}$$

where $d^2_{x_k}$ denotes the derivative of the function d^2 with respect to the variable x_k, with the boundary condition $d(x,y) = 0$ for $x = y$. Collecting terms of order δt^{-1} yields

$$-\frac{n}{2} + \frac{1}{2} L d^2 + \frac{1}{2} \sum_i \left(\sum_j \left(a_{ij}(x) + a_{ji}(x) \right) \frac{d^2_{x_j}}{2} \right) \frac{\partial c_0}{\partial x_i}(x,y) = 0, \tag{6.13}$$

where the boundary condition

$$c_0(y,y) = -\frac{1}{2} \ln \sqrt{\det \left(a_{ij}(y) \right)} \tag{6.14}$$

determines c_0 uniquely for each $y \in \mathbb{R}^n$. Finally, for $k+1 \geq 1$ we obtain

$$\begin{aligned} &(k+1) c_{k+1}(x,y) + \tfrac{1}{2} \textstyle\sum_{ij} a_{ij}(x) \left(\frac{d^2_{x_i}}{2} \frac{\partial c_{k+1}}{\partial x_j} + \frac{d^2_{x_j}}{2} \frac{\partial c_{k+1}}{\partial x_i} \right) \\ &= \tfrac{1}{2} \textstyle\sum_{ij} a_{ij}(x) \sum_{l=0}^{k} \frac{\partial c_l}{\partial x_i} \frac{\partial c_{k-l}}{\partial x_j} + \frac{1}{2} \sum_{ij} a_{ij}(x) \frac{\partial^2 c_k}{\partial x_i \partial x_j} + \sum_i b_i(x) \frac{\partial c_k}{\partial x_i}, \end{aligned} \tag{6.15}$$

with boundary conditions

$$c_{k+1}(x,y) = R_k(y,y) \text{ if } \quad x = y, \tag{6.16}$$

R_k being the right side of (6.15). In [18] it is shown how the function d^2 can be approximated in regular norms if only (WKB1) and (WKB2) are satisfied. The technique can be combined with the regular polynomial interpolations developed in [16].

6.3. *Description of algorithm (including to sparse grids and weighted Monte-Carlo versions).* We can solve (3.5), (or, similarly) (5.2) by an iterative numerical procedure.

For simplicity of description we assume that the Lipschitz constant $k \equiv k(D_t)$ of G above with respect to $|.|^D_{2,\alpha}$ is less than 1. This is true in any case for t small enough. It is clear that iteration in time of the scheme below leads to a global time scheme.

(Step1) Solve

$$\text{(6.17)}\qquad \begin{cases} u^1_{1,\tau} = \frac{1}{2}\sum_{ij} a^F_{ij}\frac{\partial^2 u^1_1}{\partial x_i \partial x_j} + \sum_j b^F_j \frac{\partial u^1_1}{\partial x_j} + r x_1 \frac{\partial u^1_1}{\partial x_1}, \\ (IC)\quad u^1_1(0,x) = \max\{K - x_1, 0\}, \end{cases}$$

where $a^1_{ij} := a^F_{ij}$ $b^1_j := b^F_j$ for $F \equiv 1$, i.e. compute

$$\text{(6.18)}\qquad u^1_1(t,x) := \int_D p_1(t,x;0,y)\max\{K - y_1, 0\}\, dy,$$

where $p_1(t,x;0,y) := p_F(t,x;0,y)$ with $F \equiv 1$.

Next solve for ϕ_1 in

$$\text{(6.19)}\qquad \begin{aligned} &\tfrac{1}{2}\phi^1(t,x) = \Gamma(t,x) + \\ &\textstyle\int_0^t \int_H (\frac{\partial}{\partial x_1} p_1(t,1,\hat{x}_1,\tau,\hat{y}_1) + p_1(t,1,\hat{x}_1;\tau,1,\hat{y}_1)) \times \\ &\phi^1(\tau,1,\hat{y}_1) dH_y d\tau, \end{aligned}$$

where $\phi^1 = \phi^F$ for $F = 1$.

Next compute

$$\text{(6.20)}\qquad u^1_2(t,\hat{x}_1) := \int_0^t \int_H p_1(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi_F(\tau,1,\hat{y}_1) dH_y d\tau$$

and

$$\text{(6.21)}\qquad F_1(t,\hat{x}_1) = K - u^1_2(t,\hat{x}_1) + u^1_1(t,x).$$

Next compute the time (first order) and spatial derivatives (up to second order) of F_1 according to the formulas (6.5) and (6.6) for $F \equiv 1$.

Remark 6.2. The use of WKB-expansions of p_1 seems the most efficient method. In [15] it was observed that a WKB approximation of the transition density including the term c_1 allows pricing of options and its derivatives with respect to the underlyings with maturity of 10 years in LIBOR models of dimension $n = 20$ with one time step (beating all concurrent methods). Moreover, efficiency and accuracy is kept for the derivatives because of explicit WKB-approximations.

(Step2) Having computed F_n For $n \geq 1$ compute F_{n+1} as follows. Compute

$$u_1^n(t,x) := \int_D p_{F_n}(t,x;0,y) \max\{K - y_1, 0\}\, dy. \tag{6.22}$$

Next solve for ϕ^n in

$$\begin{aligned} &\tfrac{1}{2}\phi^n(t,x) = \Gamma(t,x) + \\ &\int_0^t \int_H (\tfrac{\partial}{\partial x_1} p_{F_n}(t,1,\hat{x}_1,\tau,\hat{y}_1) + p_{F_n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)) \times \\ &\phi^n(\tau,1,\hat{y}_1) dH_y d\tau, \end{aligned} \tag{6.23}$$

where $\phi^n = \phi^{F_n}$.

Next compute

$$u_2^n(t,\hat{x}_1) := \int_0^t \int_H p_{F_n}(t,1,\hat{x}_1;\tau,1,\hat{y}_1)\phi^n(\tau,1,\hat{y}_1) dH_y d\tau \tag{6.24}$$

and

$$F_n(t,\hat{x}_1) = K - u_2^n(t,\hat{x}_1) + u_1^n(t,x). \tag{6.25}$$

Next compute the time (first order) and spatial derivatives (up to secons order) of F_{n+1} according to the formulas (6.5) and (6.6) for $F \equiv F_n$.

(Step3) The functions F_n form a Cauchy sequence in the Banach space $C^D_{2+\alpha}$. Hence we iterate the step 2 until

$$|F_{n+m} - F_n|^D_{2,\alpha} \leq \frac{k^n}{1-k} |F_1 - 1|^D_{2,\alpha} \leq \epsilon \tag{6.26}$$

for a prescribed $\epsilon > 0$.

REMARK 6.3. The initial step 1 and the iterated step 2 performed with WKB approximations may be done with different methods based on the dimension of the problem:

M1 For problems up to dimension 3 computation grids such as UG may be used.

M2 For higher dimensional models up to dimension $n = 5, 6$ sparse grid techniques may be used (cf. the analysis in [14] and [24]. At present -at least to my knowledge- nobody came up with stable numerical sparse grids solutions of higher dimension for linear parabolic problems with a comparable complexity.

M3 In any case Monte-Carlo realizations of the algorithmic scheme presented above are possible. Recently weighted Monte-Carlo schemes have been developed in [13] and [15], where the improved estimators established in the latter article allow also to deal with highly peaked densities which occur especially for small time or small volatility.

REMARK 6.4. For the implementation of the algorithm some recent results on regular polynomial implementation (cf. [17]) and the computation of the Riemannian metric (cf. [18]) in regular norms are needed.

REMARK 6.5. Let us look at the case of higher dimension and probabilistic realizations of the algorithmic scheme presented above. Given a free boundary approximation function F_n the Monte-Carlo estimators used for the computations of (6.22) and of (6.24) are based on the formula

$$\frac{\partial^\alpha I}{\partial x^\alpha}(x) = E\,\frac{\partial^\alpha}{\partial x^\alpha}\frac{p_{F_n}(t,x,g(x,\xi))u(g(x,\xi))}{\phi(t,x,g(x,\xi))},, \tag{6.27}$$

and $\frac{\partial^\alpha}{\partial x^\alpha}$ are spatial derivatives up to secons order or a similar formula for the time derivative. Here ξ be an $\mathbb{R}^n$-valued random variable on some probability space with a density $\lambda(z) \neq 0$ for all z, and the regular (at least twice continuously differentiable) map $\zeta^x := g(x,\xi)$ satisfies $|\partial g(x,z)/\partial z| \neq 0$, and has density $\phi(x,\cdot)$ on $\mathbb{R}^n_+$. The corresponding Monte Carlo estimator is

$$\widehat{\frac{\partial^\alpha I}{\partial x^\alpha}}(x) = \frac{1}{M}\sum_{m=1}^{M}\frac{\partial}{\partial x}\frac{p(x,g(x,_m\,\xi))u(g(x,_m\,\xi))}{\phi(x,g(x,_m\,\xi))}. \tag{6.28}$$

In [15] it is shown that the latter estimator is of bounded variance even for small time or volatility. Furthermore the extension to Bermudean options in [15] can be transferred in order to compute the Greeks for the equation (6.22). Moreover, Monte Carlo methods for computing (6.23) and (6.23) can be found in[27]

6.4. *Convergence and error analysis.* We confine ourselves to a conceptual error analysis for the higher dimensional case where the Monte-Carlo-estimators in (6.28) is used. We content ourselves with an analysis which

shows the convergence of the algorithm described above, i.e. the analysis is qualitative in the sense that the errors related to the projections of analytical approximation functions (such as WKB-expansion approximations) on grids (or sparse grids) and the numerical error induced by the computation of the Volterra integral equation are neglected. A more detailed analysis is beyond the scope of the present work and will be provided elsewhere.

The algorithm described above describes an iteration at each time step which involves the solution of an integral equation and two problems (6.22) and (6.24) both of which can be interpreted to be of parabolic first initial-boundary value problem type. For the computation of these problems we get a truncation error of the WKB-expansion and a Monte-Carlo error induced by replacing integrals by finite sums. In order to see how this turns out let

$$
\begin{aligned}
&\tfrac{\partial^\alpha I}{\partial x^\alpha}(t,x) = E\tfrac{\partial^\alpha}{\partial x^\alpha} p(t,x,\zeta)\tfrac{u(\zeta)}{\phi(t,\zeta)},\\
&\tfrac{\partial^\alpha I^{WKB,l}}{\partial x^\alpha}(t,x) = E\tfrac{\partial^\alpha}{\partial x^\alpha} p^{WKB,l}(t,x,\zeta)\tfrac{u(\zeta)}{\phi(t,\zeta)}, \text{ and}\\
&\tfrac{\partial^\alpha I}{\partial x^\alpha}(t,x) = \tfrac{1}{M}\tfrac{\partial^\alpha}{\partial x^\alpha} p^{WKB,l}(t,x,_m\zeta)\tfrac{u(_m\zeta)}{\phi(t,_m\zeta)},
\end{aligned}
\tag{6.29}
$$

where $p^{WKB,l}$ denotes the lth order WKB- approximation

$$
p_l(t,x,T,y) = \frac{1}{\sqrt{2\pi\delta t^n}}\exp\left(-\frac{d^2(x,y)}{2\delta t} + \sum_{k=0}^{l} c_k(x,y)\delta t^k\right). \tag{6.30}
$$

Then the principal error in each iteration step is estimated by

$$
\begin{aligned}
\left|\widehat{\tfrac{\partial^\alpha I}{\partial x^\alpha}}(t,x) - \tfrac{\partial^\alpha I}{\partial x^\alpha}(t,x)\right| \leq\ & \left|\widehat{\tfrac{\partial^\alpha I}{\partial x^\alpha}}(t,x) - \tfrac{\partial I^{WKB,l}}{\partial x}(t,x)\right| \\
&+ \left|\tfrac{\partial^\alpha I^{WKB,l}}{\partial x^\alpha}(x) - \tfrac{\partial^\alpha I}{\partial x^\alpha}(t,x)\right|,
\end{aligned}
\tag{6.31}
$$

leading to the error for the computation of (6.22) and (6.24). One can show that the convolution u_l of (6.30) with bounded continuous data is integrable for l large enough by comparison with the classical estimates for the Levy expansion of the fundamental solution. For large l one gets

$$
|u(t,x) - u_l(t,x)|_{1+\delta/2,2+\delta} \in O(t^{l-\frac{\delta}{2}}). \tag{6.32}
$$

using Safonov estimates cited in [19], and where u is the true value function, i.e. the convolution with the transition density p (cf. [15] for more details).

In each iteration step then we compute functions F^n and its derivatives F^n_t, $F^n_{x_i}, i \in \{2, \cdots, n\}$, and $F^n_{x_i x_j} i, j \in \{2, \cdots, n\}$ on a grid which determines the coefficient functions

$$a^{F^n_{ij}} \text{ and } b^{F^n_j}$$

on the same grid. The approximating Monte-Carlo sums then approximate the coefficients with respect to the expectation Hölder norm (cf. [15]). Next we can invoke stability results of parabolic equations with respect to coefficients and with respect to initial data for continuous affine interpolations of $a^{F^n_{ij}}$ and $b^{F^n_j}$ using the approximations on the grid points. This shows the convergence of the probabilistic scheme.

7. Epilog. We have proved regularity of the free boundary surface for a considerable class of relevant market models, and we have set up in detail a scheme for the important and difficult problem of computing the Greeks for American type options even in the context of hugher dimension. On the way we have constructed a nonlinear integral equation which characterizes the free boundary in the multivariate case. For the implementation of the scheme in more general situation an implementation of the computation of the Varadhan metric in regular norms and of the drift functions is needed. This is possible using regular polynomial interpolation (cf. [16] and the analysis of the eikonal equation characterizing the Varadhan metric global approximation of its solution (cf. [18]). The scheme established is very flexible. Note that PDE-scheme realizations are possible beside Monte-carlo realizations especially for lower-dimensional models. Detailed error analysis for different realizations of the scheme and their implementations is certainly of interest. Furthermore, extension to jump-diffusion models is possible and will be considered elsewhere.

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