

The world is continuous, but the mind is discrete.

David Mumford (ICM 2002 plenary talk, Aug. 21, 2002).

Abstract

Modern finite difference schemes usually try to accomplish the following goals: (i) the scheme must be at least of second order of approximation in all independent variables; (ii) it should be unconditionally stable; (iii) it should preserve nonnegativity of the solution. Here we give the main definitions and facts of the modern theory of finite difference schemes using an operator approach to the solution of a parabolic partial differential equations or partial integrodifferential equations and Padé approximations. We also introduce operator splitting techniques and high-order compact (HOC) schemes. In an appendix, some examples of HOC schemes are provided as applied to pricing American options.

2.1 Introduction

In this book we focus on Markovian financial models used for pricing derivatives for various asset classes. Using a standard approach of mathematical finance, this problem can be eventually translated to the solution of some partial differential equation (PDEs) or partial integrodifferential equations (PIDEs). As a simple example, let us consider a parabolic PDE written in a general form

$$\frac{\partial V(\mathbf{x}, \tau)}{\partial \tau} = \mathcal{L}V(\mathbf{x}, \tau), \quad V(\mathbf{x}, 0) = V_0(\mathbf{x}) \quad (2.1)$$

given some boundary conditions at the boundary of the domain where \mathbf{x} is defined. In Eq. (2.1), τ is time, \mathbf{x} is a vector of spatial independent variables, $V(\mathbf{x}, \tau)$ is the dependent variable and \mathcal{L} is a spatial (parabolic) operator. For instance, in the celebrated Black–Scholes model [21], $V(x, \tau)$ can be seen as the European vanilla call option price, $x = \log S$, S is the underlying spot price, τ now becomes the backward time, e.g., $\tau = T - t$, where t is the calendar time and T is the time to expiration (maturity), while

$$\mathcal{L} = \left(r - q - \frac{1}{2}\sigma^2 \right) \frac{\partial}{\partial x} + \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} - r, \quad (2.2)$$

with r, q are the interest and continuous dividend rates, respectively, and σ the volatility.

Formal integration of Eq. (2.1) in this one-dimensional case gives rise to the solution

$$V(x, \tau) = e^{\tau \mathcal{L}} V(x, 0). \quad (2.3)$$

Here $e^{\tau \mathcal{L}}$ is the operator exponential, which acts exactly like the Taylor series expansion of $e^{\tau L}$ around $\tau = 0$.

This representation, however, is not correct if $\mathcal{L} = \mathcal{L}(\tau)$. For instance, in some models, r and σ could be assumed to be deterministic functions of t . In this case, one can approximate such a dependence by a piecewise constant function, so that at each time interval $\Delta\tau_i = \tau_i - \tau_{i-1}$, we have $r = r(\tau_i), \forall \tau \in [\tau_{i-1}, \tau_i]$ and $\sigma = \sigma(\tau_i), \forall \tau \in [\tau_{i-1}, \tau_i]$. Then, similar to Eq. (2.10), for the i th time interval we can write

$$V(x, \tau_i + \Delta\tau_i) = e^{\Delta\tau_i \mathcal{L}} V(x, \tau_i). \quad (2.4)$$

In doing so, we obviously introduce an error by approximating the continuous coefficients of the operator \mathcal{L} with piecewise constant functions that have order $O(\Delta\tau)$. But once the assumption of piecewise constancy is made, the solution Eq. (2.4) is still exact on the time interval $(\tau_{i-1}, \tau_i]$, e.g., no additional discretization in x or $\Delta\tau$ of the solution has been performed so far.

For the sake of simplicity, in the remaining part of this section we consider $\Delta\tau_i \equiv \Delta\tau$, i.e., a uniform temporal grid. This, however, doesn't bring any limitation on our further description, and this assumption can be easily relaxed.

Although the representation Eq. (2.4) is an exact solution, it cannot be obtained in an explicit form in the general case. Therefore, to get an approximate solution we use the finite difference method, which is our method of choice.

To explain this, let us recall that this book is dedicated to pricing financial derivatives using Lévy processes. Multidimensional Lévy processes find various applications in mathematical finance. They are used in modeling basket equity derivatives, various credit derivatives, and so on. Unfortunately, the tractability of multidimensional Lévy processes is rather limited. In addition, it is difficult to study such processes because they suffer from the curse of dimensionality. Various numerical methods, including analytical, semianalytical, finite difference, Monte Carlo, and their combinations have been used for

solving such problems; see, e.g., the survey in [31] and references therein. Certainly, a Monte Carlo method can be proposed to simulate multidimensional Lévy processes. However, unless special care is taken, a generic method is both slow and inaccurate. Moreover, since in most situations neither the PDF nor the CDF of a multidimensional Lévy process is known, some extensions of the Monte Carlo method should be used that combine the standard Monte Carlo approach with Fourier inversion; see, for instance, [3]. Therefore, finite difference methods seem to be a preferred alternative, at least for 2D and 3D problems.

As far as the finite element method is concerned, in some sense it is similar to the FD method. In the following chapters, in discussing solutions of some particular problems, we provide necessary references to the existing literature on the finite element approach and to various existing implementations. However, the main goal of this book is to present a new method of pseudodifferential operators for efficiently solving PIDEs for various Lévy jump models. Perhaps the idea of that approach could be further extended to substitute the FD method with its FEM counterpart. This could be a subject of future research.

In solving Eq. (2.4) numerically using the FD method, we can either discretize the operator \mathcal{L} (which should be done on some spatial grid in \mathbf{x}) or use a temporal discretization of the matrix exponential $e^{\Delta\tau\mathcal{L}}$ in Δ , τ , or both. In the next section we consider all these types of discretizations.

However, before doing so, let us also note that the transition operator (matrix exponential) on the right-hand side of Eq. (2.4) can also be efficiently computed using a direct approach. The existing methods of computing the matrix exponential basically use Padé approximations with scaling and squaring; see [34] and references therein, and also [43]. However, the complexity of computing a general Padé approximant is $O(N^3)$, which is slow. Therefore, the researchers sought to provide some better methods. One of the most promising techniques uses the best rational approximation via Carathéodory–Fejér (CFE) points, as was proposed in [39, 46]. It gives a rational approximation to the operator $e^{\mathcal{L}}$ as the expansion (see also [43])

$$e^{\mathcal{L}} = \sum_{j=1}^{\eta} b_j (\mathcal{L} - z_j I)^{-1}, \quad (2.5)$$

where the residues b_j and poles z_j are tabulated as in [5]. Here η represents the number of CFE points taken, and the error of the above rational approximation decays exponentially with asymptotic behavior $O(9.28903^{-\eta})$ [15].

Therefore, as will be shown in Section 2.3, if the operator \mathcal{L} is discretized on some grid, and after that the matrix of the discrete operator L is banded, the representation Eq. (2.5) provides an efficient way of computing the matrix exponential with high accuracy by solving a set of systems of linear equations with banded matrices. Also, since the matrices that arise in financial problems are real, the poles and residues come in complex conjugate pairs. Thus, only 0.5η shifted linear systems have to be solved, making the rational approximation very efficient. For further details, see [43].

2.2 Discretization of $e^{4\tau\mathcal{L}}$ on a Temporal Grid

If we don't need the exact solution of Eq. (2.1) in time (which can be time-consuming to obtain), but only the solution up to some accuracy in $\Delta\tau$, then the exponent on the right-hand side of Eq. (2.4) can be substituted with its discrete approximation. The beauty of the representation Eq. (2.4) lies in the fact that all classical FD schemes can be obtained from Eq. (2.4) using a technique of Padé approximants.

The technique was developed around 1890 by Henri Padé but actually goes back to Ferdinand Georg Frobenius, who introduced the idea of rational approximations of power series [14].

Definition 2.1. Given a function $f(x)$, $x \in \mathbb{R}$, and two integers $m \geq 0$ and $n \geq 1$, the Padé approximant of order (m, n) is the rational function

$$R(x) = \frac{\sum_{j=0}^m a_j x^j}{1 + \sum_{k=1}^n b_k x^k} = \frac{a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m}{1 + b_1 x + b_2 x^2 + \cdots + b_n x^n},$$

such that

$$f(x) - R(x) = c_{m+n+1} x^{m+n+1} + c_{m+n+2} x^{m+n+2} + \cdots = O(x^{m+n+1}).$$

It can be shown [14] that given m and n , the Padé approximant is unique, which means that the coefficients $a_0, a_1, \dots, a_m, b_1, \dots, b_n$ can be uniquely determined. It is for reasons of uniqueness that the zeroth-order term in the denominator of $R(x)$ was chosen to be 1; otherwise, the numerator and denominator of $R(x)$ would have been unique only up to multiplication by a constant.

Under some mild assumptions on the existence, Definition 2.1 can be extended to cover not only the functions but also the operators; see, e.g., [12, 47]. Accordingly, various FD schemes can be obtained by choosing Padé approximations of the operator exponential with some orders m, n .

2.2.1 Examples

Explicit Euler scheme.

Using the $(1, 0)$ Padé approximation of e^x , from Eq. (2.4) we get

$$V(x, \tau + \Delta\tau) = (1 + \Delta\tau\mathcal{L})V(x, \tau) + O(\Delta\tau). \quad (2.6)$$

This can be easily recognized as an explicit Euler scheme [9]. It is known that this scheme is only conditionally stable (see below), and therefore is of limited use in practice. Also, it is only of first order of approximation in $\Delta\tau$.

Implicit Euler scheme.

Using the (0, 1) Padé approximation of e^x , from Eq. (2.4) we get

$$V(x, \tau + \Delta\tau) = (1 - \Delta\tau\mathcal{L})^{-1}V(x, \tau) + O(\Delta\tau),$$

or, rearranging terms,

$$(1 - \Delta\tau\mathcal{L})V(x, \tau + \Delta\tau) = V(x, \tau) + O(\Delta\tau). \quad (2.7)$$

This is an FD implicit Euler scheme [9]. It is known that this scheme is unconditionally stable (also see below), while it provides only the first order of approximation in $\Delta\tau$.

Crank–Nicolson scheme.

Using the (1, 1) Padé approximation of e^x , from Eq. (2.4) we get

$$\left(1 - \frac{1}{2}\Delta\tau\mathcal{L}\right)V(x, \tau + \Delta\tau) = \left(1 + \frac{1}{2}\Delta\tau\mathcal{L}\right)V(x, \tau) + O((\Delta\tau)^2). \quad (2.8)$$

This is a familiar Crank–Nicolson scheme [9]. It is A-stable (see below) and provides the second order of approximation in $\Delta\tau$.

However, it is known that the diagonal Padé schemes, to which the CN scheme belongs, are susceptible to oscillations when high-frequency components are present, since their symbols have unit magnitude at infinity; see [47] for definitions and also references therein. Usually, low-order schemes require some additional smoothing or damping to preserve oscillations, if not in the solution itself, then in the derivatives. Also, discontinuous initial (payoff) or boundary (discrete monitoring) conditions cause damping problems for this kind of FD scheme [35]. Therefore, in [47] it is proposed to use high-order nondiagonal Padé approximations, which have better damping properties and also have nice positivity properties. We send the reader to the cited paper for further details. Nevertheless, let us give an example of a fourth-order scheme that reads

$$V(x, \Delta\tau) = \left(1 + \Delta\tau\mathcal{L} + \frac{1}{2}\Delta\tau^2\mathcal{L}^2 + \frac{1}{6}\Delta\tau^3\mathcal{L}^3\right)V(x, 0) \quad (2.9)$$

$$V(x, 2\Delta\tau) = \left(1 + \Delta\tau\mathcal{L} + \frac{1}{2}\Delta\tau^2\mathcal{L}^2 + \frac{1}{6}\Delta\tau^3\mathcal{L}^3\right)V(x, \Delta\tau)$$

$$\left(1 - \Delta\tau\mathcal{L} + \frac{1}{12}\Delta\tau^2\mathcal{L}^2\right)V(x, \tau + \Delta\tau) = \left(1 + \Delta\tau\mathcal{L} + \frac{1}{12}\Delta\tau^2\mathcal{L}^2\right)V(x, \tau),$$

$$\tau \geq 2\Delta\tau.$$

The operator $\mathcal{M} = 1 - \Delta\tau\mathcal{L} + \frac{1}{12}\Delta\tau^2\mathcal{L}^2$ can be further factorized into the product

$$\mathcal{M} = \frac{1}{12}(a_1 - \Delta\tau\mathcal{L})(a_2 - \Delta\tau\mathcal{L}), \quad a_1 = 6 - 2\sqrt{6}, \quad a_2 = 2(3 + \sqrt{6}).$$

So the solution of the last line in Eq. (2.9) could be done in two sequential steps. However, for some Padé FD schemes obtained in a similar way, the coefficients a_i can be complex. Hence, the complexity of obtaining the whole solution increases.

2.3 Discretization of the Operator \mathcal{L} on a Spatial Grid

To build a discrete version of the exponent in Eq. (2.4), an appropriate discrete grid $\mathbf{G}(x)$ has to be constructed in the domain of definition of \mathbf{x} . If this domain is of infinite size (for instance, in pricing European vanilla options, the domain for the stock price S is semi-infinite), it has to be truncated based on some additional consideration, for instance, to fit the memory and performance requirements. Also, this grid could be either uniform or nonuniform. After discretization is done, the continuous equation Eq. (2.3) should be substituted with its discrete approximation, which reads

$$C(x, \tau) = e^{\tau L} C(x, 0), \quad (2.10)$$

where L is now a matrix representing a discrete approximation of \mathcal{L} on $\mathbf{G}(x)$, C is a vector of solutions that approximates $V(\mathbf{x}, \tau)$ on $\mathbf{G}(x)$, and x is a vector of the grid nodes. For the sake of simplicity, we use the same notation for x in both continuous and discrete cases, since it should not cause any ambiguity.

2.3.1 Uniform Grid

The size of the grid in space must be chosen based on the appropriate boundary conditions. For instance, in pricing an American option written on a single stock or an index, one boundary condition is set at $S = 0$. So this point is a natural choice for the lower grid boundary. The second boundary condition is set at $S \rightarrow \infty$. If we don't use any analytic transformation to move this point from infinity to some fixed point, the infinite domain must be truncated to some $S = S_{\max}$. The value of S_{\max} must be chosen "as large as possible." For a numerical scheme, this can be problematic, since the number of grid points may grow very large. In [27], the proper size of the domain is proposed after a careful analysis. For instance, for the Black–Scholes equation, the far field boundary reads

$$S_{\max} = \max \left[2K, K \exp \left(\sigma \sqrt{2T \ln 100} \right) \right], \quad (2.11)$$

where K is the strike. This expression works well for a single strike K . However, if one wants to use it to get the option prices for several strikes, an appropriate upper boundary suitable for doing so for the whole range of the considered strikes has to be chosen. Also, in this case, the implied volatility σ is usually taken from the volatility smile curve, and therefore is a function of the strike. Thus, instead we have to use the similar expression

$$S_{\max} = \max_K \left\{ \max \left[2K, K \exp \left(\sigma(K) \sqrt{2T \ln K / \Delta} \right) \right] \right\}, \quad (2.12)$$

where Δ is that absolute accuracy in S that we want to achieve, and the maximum is taken over the whole range of the traded option strikes given the name and expiration. This increases the grid size by several times, but this could be partly compensated by using a nonuniform space step.

Certainly, for financial instruments similar, e.g., to a double barrier option, the spatial domain is naturally defined by the contract definition.

Once a particular choice of the lower x_0 and upper x_n boundaries is made for the given problem, so that $x \in [x_0, x_n]$, $x_0 > -\infty$, $x_n < \infty$, a certain uniform grid can be constructed with $n + 1$ nodes (x_0, x_1, \dots, x_n) and spatial steps $h_i = x_i - x_{i-1} \equiv h$, $i \in [1, n]$, such that $x_n = x_0 + nh$.

We now introduce some definitions. Below, for sake of convenience we denote an operator of the first derivative ∂_x by ∇ .

Definition 2.2. Define a one-sided *forward* discretization of ∇ , which we denote by A^F : $A^F C(x) = [C(x + h, t) - C(x, t)]/h$. Also define a one-sided *backward* discretization of ∇ , denoted by A^B : $A^B C(x) = [C(x, t) - C(x - h, t)]/h$. These discretizations provide a first-order approximation in h , e.g., $\nabla C(x) = A^F C(x) + O(h)$.

Definition 2.3. Define $A_2^C = A^F A^B$, the *central* difference approximation of the second derivative $\nabla^2 \equiv \partial_{x,x}$, and $A^C = (A^F + A^B)/2$, the *central* difference approximation of the first derivative ∇ . Also define a one-sided second-order approximation to the first derivatives: *backward* approximation A_2^B : $A_2^B C(x) = [3C(x) - 4C(x-h) + C(x-2h)]/(2h)$, and *forward* approximation A_2^F : $A_2^F C(x) = [-3C(x) + 4C(x+h) - C(x+2h)]/(2h)$. All these approximations are of second order in the spatial step h .

In what follows, we will denote the identity matrix by I .

2.3.2 Nonuniform Grid

A uniform grid has many disadvantages, especially for problems in which the gradient of the solution greatly changes its magnitude across the spatial domain, or either the solution itself or its derivatives have discontinuities, for instance close to the option strike K or to

the barrier. That is because the solution Eq. (2.4) is very sensitive to localization errors when S is in the vicinity of K , or close to the barrier, since the first derivative of the payoff doesn't exist at this point. Obviously, for any FD scheme it is difficult to resolve this discontinuity or a possible jump in the solution value due to high gradients within just few FD cells.

Therefore, to increase accuracy, it would be reasonable to use an adaptive mesh with a high concentration of the mesh points around $S = K$, while a rarefied mesh could be used far away from this area. For barrier options, the situation is even more complicated [45]. Here we consider only continuously sampled barriers, so it is sufficient to place the barriers on the boundaries of the grid and enforce a boundary condition. This boundary condition is determined by definition of the contract, and, e.g., could be that the option expires worthless or rebate is paid when the stock price hits the barrier. The gradient of the option price is discontinuous at the barriers, because we never solve the pricing equation there. Therefore, it is reasonable to concentrate the grid cells in the vicinity of the barriers as well.¹

For multidimensional problems, e.g., in solving a 2D PDE arising under stochastic volatility models, it is reasonable to compress the 2D grid close to the peculiarities (e.g., areas where the solution has high gradients) of the solution in both directions. For instance, for the Heston model it makes sense to concentrate the mesh points close to $S = K$ and $v = 0$ [23], where v is the instantaneous variance. This greatly improves the accuracy of the scheme as compared to uniform meshes. Also, at $v = 0$, the PDE becomes convection dominated, so it is reasonable to concentrate meshes at this point as well as at the initial level of v .

There are several approaches to building a nonuniform grid. Let us consider two of them.

Coordinate transformation.

If the desired nonuniform grid is expected to condense the mesh points in the vicinity of more than just one critical point, then it makes sense to apply a coordinate transformation to the original PDE. Following [25, 45], consider a problem of pricing a double barrier European call option under the Heston model. In this model, the spot volatility is assumed to be a stochastic variable, and Heston [18] suggested to model it as a square-root process. Therefore, the dynamics of the underlying stochastic drivers in the Heston model reads

$$\begin{aligned} dS_t &= S_t(r - q)\mu dt + S_t\sqrt{v_t}dW^{(1)} \\ dv_t &= \kappa(\theta - v_t)dt + \xi\sqrt{v_t}dW^{(2)}, \\ S_t|_{t=0} &= S_0, \quad v_t|_{t=0} = v_0, \end{aligned} \tag{2.13}$$

¹For sampling barriers discretely, this could result in some problems; see the discussion in [45].

where $W^{(1)}$ and $W^{(2)}$ are correlated Brownian motions with constant correlation coefficient ρ , κ is the rate of mean reversion, ξ is the volatility of the variance v , θ is a mean-reversion level (long-term run value). All parameters in the Heston model are assumed to be time-independent.

Every contingent claim $V(t, S, v)$ paying at maturity T the payoff $g(S)$ solves the PDE [13]

$$\begin{aligned} \frac{\partial}{\partial \tau} V(\tau, S, v) = & -rV(\tau, S, v) + (r - q)S \frac{\partial}{\partial S} V(\tau, S, v) + \kappa(\theta - v) \frac{\partial}{\partial v} V(\tau, S, v) \\ & + \frac{1}{2} v S^2 \frac{\partial^2}{\partial S^2} V(\tau, S, v) + \frac{1}{2} \xi^2 v \frac{\partial^2}{\partial v^2} V(\tau, S, v) + \rho \xi v S \frac{\partial^2}{\partial S \partial v} V(\tau, S, v), \quad (2.14) \\ V(0, S, v) = & g(S), \quad V(\tau, L_b, v) = V(\tau, H_b, v) = 0, \end{aligned}$$

where L_b, H_b are respectively the lower and upper barriers.

Let us make a transformation of independent coordinates (x, v) such that we transform the coordinate $x = \log S$ independently of the other coordinate. In other words, we use a map $x \leftrightarrow X, v \leftrightarrow V$ of the form

$$x = x(X), \quad v = V(v). \quad (2.15)$$

Next we use a transformation that has been proposed in [45] with the idea of concentrating the FD mesh points near the critical points such as the barriers and the strike. We define the Jacobian of this transformation as

$$J(X) = \frac{dx(X)}{dX}, \quad (2.16)$$

where

$$\begin{aligned} J(X) = & A \left[\sum_{k=1}^{k=3} J_k(X)^{-2} \right]^{-1/2} \quad (2.17) \\ J_k(X) = & [\alpha_k^2 + (x(X) - B_k)^2]^{1/2} \end{aligned}$$

The parameters B_k correspond to the critical points, i.e., in our case, $B_1 = \log L_b$, $B_2 = \log H_b$, $B_3 = \log K$. The parameters A and $\alpha_k, k = 1, 2, 3$, are adjustable. Setting $\alpha_k \ll B_2 - B_1$ yields a highly nonuniform grid, while $\alpha_k \gg B_2 - B_1$ yields a uniform grid.

For the transformation given by Eq. (2.17), the global Jacobian $J(X)$ near the strike and the barriers is dominated by the behavior of the local $J_k(X)$, but the influence of nearby critical points ensures that the transitions between them are smooth. In general, the global Jacobian must be integrated numerically to yield the transformation $x(X)$. Any standard ODE integrator (for instance, Matlab ode45) could be used for that, using the

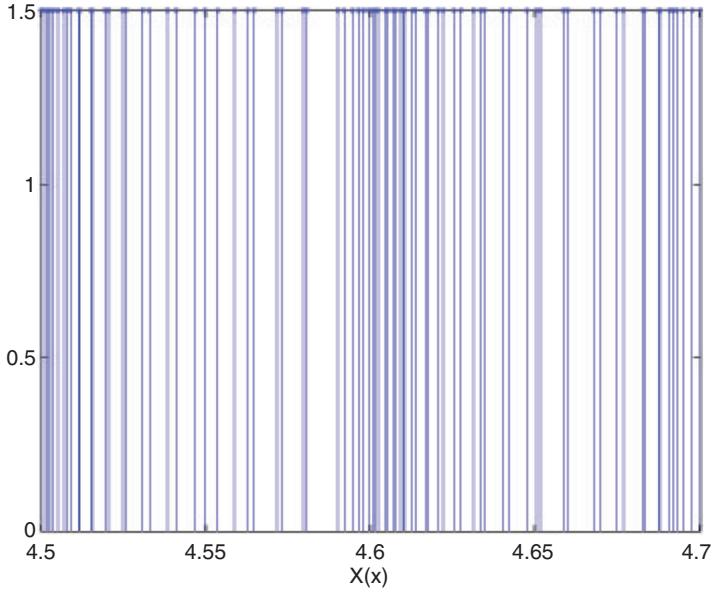


Fig. 2.1 New grid obtained from the uniform grid in x with the transformation Eq. (2.17)

initial condition $x(0) = B_1$. The second boundary condition connects the points B_2 on the original grid and $\log X_{\max}$ on the transformed grid. The value of X_{\max} , the right end of the X -grid, can be chosen arbitrarily, for instance $X_{\max} = 1$. Thus, to satisfy the condition $x(X_{\max}) = B_2$, one can vary the adjustable parameter A . Since $x(X_{\max})$ is monotonically increasing with A , the numerical iterations are guaranteed to converge.

In Fig. 2.1, we present a map of the new grid obtained in [25] by transforming the original grid uniform in x with the transformation Eq. (2.17). The new grid in x contains 41 nodes distributed from $\log L_B$ to $\log H_B$. The values of the parameters used in this example are $H = 110, L = 90, K = 100, \alpha_H = \alpha_L = (\log H_B - \log L_B)/30, \alpha_K = (\log H_B - \log K)/10$.

Note that for the transformation Eq. (2.17),

$$\begin{aligned} \frac{d \ln J(x)}{dx} &= \frac{dJ}{dx} = A \left\{ \sum_{k=1}^3 \frac{x - B_k}{[\alpha_k^2 + (x - B_k)^2]^2} \right\} \left[\sum_{k=1}^3 \frac{1}{\alpha_k^2 + (x - B_k)^2} \right]^{-3/2} \\ &\approx A \left[\frac{1}{(x - \log H_B)^3} + \frac{1}{(x - \log K)^3} + \frac{1}{(x - \log L_B)^3} \right] \cdot \\ &\quad \left[\frac{1}{(x - \log H_B)^2} + \frac{1}{(x - \log K)^2} + \frac{1}{(x - \log L_B)^2} \right]^{-3/2}. \end{aligned} \quad (2.18)$$

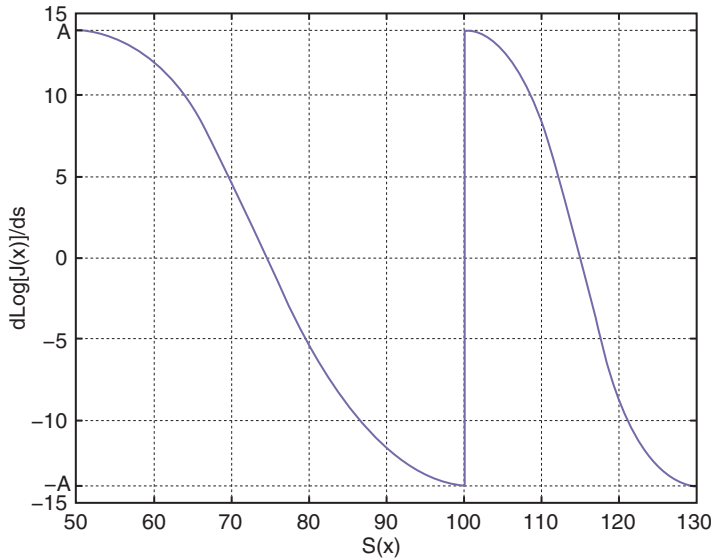


Fig. 2.2 $d \ln J(X)/dX$ as a function of $S(X)$. The parameters for this test are given after Fig. 2.1, while the barriers are moved to $H_B = 130, L_B = 50$

This function is bounded and changes within the range $(-A, A)$, as can be seen in Fig. 2.2. Thus $|d \ln J(x)/dx|$ is bounded.

To preserve monotonicity of the grid as well as monotonicity of the grid steps h_i , $i = 1, N$, after A and the Jacobian are computed, in [25] an additional grid smoothing is applied by running a robust local regression with a moving average. The latter uses weighted linear least squares and a second-degree polynomial model. So the new grid steps are s_i , $i = 1, N$. After this step is complete, the grid is renormalized to have it fit the original boundaries. In other words, we compute a constant R : $R = \sum_i h_i / \sum_i s_i$ and then reassign $h_i = R s_i$, $i = 1, n$. The span for the moving average is equal to 10.

Moving on to the second variable v , in [25] the same type of transformation is used as in Eq. (2.17), where now the critical points $B_1 = 0$ and $B_2 = v_0$ are considered. In Fig. 2.3, a map $X - V$ of the new grid obtained from the original uniform 2D $x - v$ grid using the transformation Eq. (2.17) is depicted. The new grid contains 101 nodes in X distributed from $\log L_B$ to $\log H_B$, and 61 nodes in V distributed from 0 to V_{\max} . The values of the parameters used in this example are $H_b = 110, L_B = 90, K = 100, \alpha_H = \alpha_L = (\log H_B - \log L_B)/60, \alpha_K = (\log H_B - \log K)/20, \alpha_0 = \alpha_{v_0} = V_{\max}/20$; and $V_{\max} = 1.5$ is the maximum value of V on the grid.

Condensing mesh around a single point.

An alternative approach when the grid contains just a single critical point is described, e.g., in [16, 23, 45]. In the x -direction, a relatively large number of mesh points are placed throughout a given interval $[S_l, S_r]$, $S_l < K < S_r$, $[S_l, S_r] \subset [0, x_{\max}]$. This is natural,

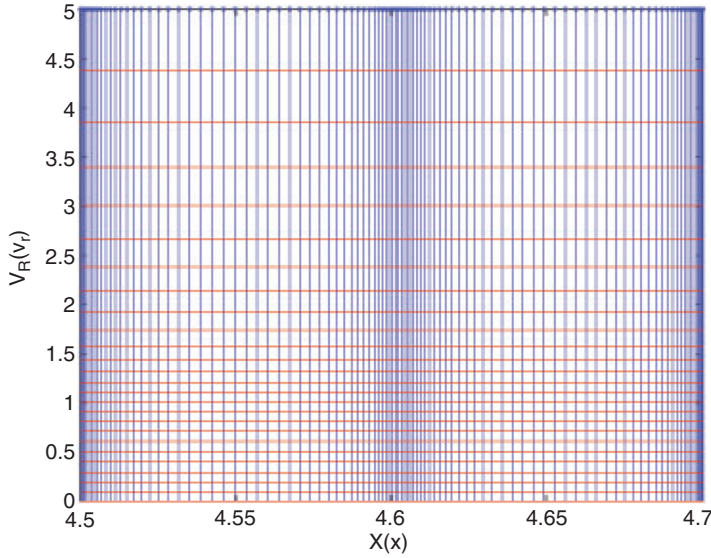


Fig. 2.3 New grid obtained from the uniform grid in x, v with the transformation Eq. (2.17)

because this is the region of interest in applications, and also it alleviates numerical difficulties due to the discontinuity of the payoff function at $S = K$. Define the integer $m_1 = 1$ and the parameter $d_1 > 0$, and let equidistant points $\xi_{\min} = \xi_0 < \xi_1 < \dots < \xi_m = \xi_{\max}$ be given with

$$\begin{aligned}\xi_{\min} &= \sinh^{-1} \left(-\frac{S_l}{d_1} \right), \\ \xi_{int} &= \frac{S_r - S_l}{d_1}, \\ \xi_{\max} &= \xi_{int} + \sinh^{-1} \left(\frac{S_{\max} - S_r}{d_1} \right).\end{aligned}\tag{2.19}$$

As can be seen, $\xi_{\min} < 0 < \xi_{int} < \xi_{\max}$. The mesh $0 = S_0 < S_1 < \dots < S_{m_1} = S_{\max}$ is then defined through the transformation

$$S_i = \phi(\xi_i), \quad 0 \leq i \leq m_1,\tag{2.20}$$

where

$$\phi(\xi) = \begin{cases} S_l + d_1 \sinh(\xi), & \xi_{\min} \leq \xi \leq 0, \\ S_l + d_1 \xi, & 0 \leq \xi \leq \xi_{int}, \\ S_r + d_1 \sinh(\xi - \xi_{int}), & \xi_{int} < \xi \leq \xi_{\max}. \end{cases}\tag{2.21}$$

This mesh is uniform in S inside the interval $[S_l, S_r]$, and it is nonuniform outside this interval. The parameter d_1 controls the fraction of points S_i that lie inside. As shown in [16], the above mesh is smooth, in the sense that there exist real constants C_0, C_1, C_2 such that the mesh widths $h_i = S_i - S_{i-1}$ satisfy

$$C_0 h \leq h_i \leq C_1 h, \quad |h_{i+1} - h_i| \leq C_2 h^2, \quad h = \xi_1 - \xi_0$$

uniformly in i, m_1 .

Approximation of derivatives.

Once a nonuniform grid is constructed, the first and second derivatives can be approximated on this grid. The corresponding expressions are obtained using Taylor series expansions. Here for reference we provide just the final results; see, e.g., [16, 23].

Definition 2.4. Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be any given function, let $x_i, i \in \mathbb{Z}$, be any given increasing sequence of mesh points, and let $h_i = x_i - x_{i-1}, \forall i$. To approximate the first derivatives of $f(x)$, employ the following FD formulas.

Backward scheme:

$$D_{2B}^1 = \alpha_{-2}f(x_{i-2}) + \alpha_{-1}f(x_{i-1}) + \alpha_0f(x_i) = \nabla f(x_i) + O((h_i + h_{i-1})^2).$$

Forward scheme:

$$D_{2F}^1 = \gamma_0f(x_i) + \gamma_1f(x_{i+1}) + \gamma_2f(x_{i+2}) = \nabla f(x_i) + O((h_{i+1} + h_{i+2})^2).$$

Central scheme:

$$D_{2C}^1 = \beta_{-1}f(x_{i-1}) + \beta_0f(x_i) + \beta_1f(x_{i+1}) = \nabla f(x_i) + O((h_i + h_{i+1})^2).$$

Here

$$\begin{aligned} \alpha_{-2} &= \frac{h_i}{h_{i-1}(h_i + h_{i-1})}, & \alpha_{-1} &= -\frac{h_{i-1} + h_i}{h_i h_{i-1}}, & \alpha_0 &= \frac{h_{i-1} + 2h_i}{h_i(h_{i-1} + h_i)}, \\ \gamma_0 &= -\frac{2h_{i+1} + h_{i+2}}{h_{i+2}(h_{i+2} + h_{i+1})}, & \gamma_1 &= \frac{h_{i+2} + h_{i+1}}{h_{i+2}h_{i+1}}, & \gamma_2 &= -\frac{h_{i+1}}{h_{i+2}(h_{i+2} + h_{i+1})}, \\ \beta_{-1} &= -\frac{h_{i+1}}{h_i(h_{i+1} + h_i)}, & \beta_0 &= \frac{h_{i+1} - h_i}{h_{i+1}h_i}, & \beta_1 &= \frac{h_i}{h_{i+1}(h_{i+1} + h_i)}. \end{aligned}$$

Definition 2.5. Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be any given function, let $x_i, i \in \mathbb{Z}$, be any given increasing sequence of mesh points, and $h_i = x_i - x_{i-1}, \forall i$. To approximate the second derivatives of $f(x)$ employ the following FD formulas.

Central scheme:

$$D_{2C}^2 = \delta_{-1}f(x_{i-1}) + \delta_0f(x_i) + \delta_1f(x_{i+1}) = \nabla^2f(x_i) + O((h_i + h_{i+1})^2).$$

Here

$$\delta_{-1} = \frac{2}{h_i(h_{i+1} + h_i)}, \quad \delta_0 = -\frac{2}{h_{i+1}h_i}, \quad \delta_1 = \frac{2}{h_{i+1}(h_{i+1} + h_i)}.$$

Let $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ be any given function of two variables (x, y) . To approximate the mixed derivative $\nabla_x \nabla_y f(x_i, y_j)$ at any point (x_i, y_j) , one can apply either one-sided approximations in each direction or apply the central difference approximation first in x and then in y (or vice versa). The latter results in the FD approximation of the mixed derivative using a nine-point stencil while still providing a second-order approximation. We will discuss this and other possible approximations in more detail in the next chapter, in Section 3.4.

2.4 Requirements of Modern FD Schemes

Modern FD schemes are widely used in financial mathematics to solve numerically various types of PDE and PIDE. Usually, this is necessary in pricing certain financial instruments, so that the corresponding price is given by the solution of the corresponding PDE/PIDE. Accordingly, calibration of these financial models is also provided by the pricing method of choice. This dictates certain requirements regarding the quality of the FD scheme used in finance. Certainly, under scrutiny, they could differ based on the asset class to which the considered derivative belongs, or on some peculiarities of the corresponding market. Nevertheless, it is possible to formulate some general requirements for the FD schemes that seem to be rather common in modern financial mathematics. Hence, a majority of researchers, financial software vendors, and developers of pricing libraries in various banks and investment firms are trying to follow them. Below, we briefly discuss these requirements and also introduce the main definitions and references to the existing literature. Then in Section 3, we will consider them again to reformulate them in terms of an M-matrix theory.

2.4.1 Order of Approximation

In looking at various possible temporal and spatial discretizations of the PDE Eq. (2.1) presented in the previous section, a natural question is to determine the orders of approximation in both time and space that are practical for financial problems. In principle, the answer could depend on certain characteristics of the financial instrument under

consideration, such as the particular market, whether you need the method for pricing, and the calibration or calculation of certain risk characteristics of the given portfolio. In general, the modern trend is to use FD schemes at least of second order of approximation in both space and time. However, as was already mentioned, higher accuracy usually results in degradation of performance. Therefore, for calibration of some model using the FD approach, it might be reasonable to use a lower-order scheme to provide better performance. At the very least, the results obtained in such a way can be considered a good initial guess for running a more accurate calibration algorithm.

At the same time, some higher-order schemes have been widely reported in the literature as being used just for accurate pricing. Note that a higher order of approximation can be achieved by expanding the FD stencil, i.e., using higher-order approximations for the first and the second derivatives, which involves more grid points per derivative. This is not an optimal approach, since the complexity of the calculations increases accordingly. Therefore, significant errors were made in building higher-order approximations in the class of so-called HOC (high-order compact) schemes [44], which provide a higher order of approximation on the same stencil.

In place of a detailed discussion, let us just mention that for an accurate pricing of options in market making or options trading, the modern requirements are to get these prices with an absolute accuracy better than half a cent. For equity options written on some stock whose price is, e.g., \$500, this absolute accuracy translates to a relative error of 10^{-5} , while the size of the FD grid should be kept relatively medium. To achieve this, we need in general to work with an HOC scheme, sometimes of fourth order in space $O(h^4)$ or even better. On the other hand, a high-order approximation in time would also be very desirable. As shown in [44], the HOC scheme for the heat equation with smooth initial conditions attains clear fourth-order convergence but fails if nonsmooth payoff conditions are used. Therefore, it is impossible to resolve this problem using just an HOC scheme in space as some authors have claimed.

For homogeneous parabolic partial differential equations with nonsmooth initial data, a family of smoothing schemes with higher-order accuracy has recently been developed (see the literature survey in [28]). Convergence results and numerical experiments show that these schemes can be more robust than the well-known Rannacher smoothing schemes [37] with respect to spurious oscillations generated through high-frequency components in nonsmooth initial or boundary data. These schemes are usually constructed based on Padé approximation of the evolutionary operator, similar to what we discussed in Section 2.2. Unfortunately, to the best of our knowledge, these schemes operate mostly with a second-order discretization in space. Using an HOC scheme in space together with the Padé scheme brings some extra complexity. So if someone were looking for a speedy implementation of a pricing algorithm, perhaps, she would prefer to eliminate this approach. The other problem is that for the Padé scheme to be efficient, it should be parallelized, which in general, results in the necessity to work with complex arithmetic; see, e.g., [47]. Fortunately, many standard libraries, e.g., the CUBLAS library for CUDA, support complex arithmetic, and therefore, working with HOC Padé schemes could be a possible challenge.

In the appendix to this chapter we describe some example of HOC schemes defined on a uniform grid used for pricing American options. These examples are provided basically with a pedagogical purpose to familiarize the reader with this technique. A more sophisticated approach to constructing HOC schemes for pricing equity options can be found in [44].

2.4.2 Stability

In the mathematical subfield of numerical analysis, numerical stability is generally a desirable property of a numerical algorithm. As applied to iterative procedures, like the FD schemes, it has been observed that some numerical algorithms may damp out small fluctuations (errors) in the input data. Others might magnify such errors. Calculations that can be proven not to magnify approximation errors are called numerically stable. One of the common tasks of numerical analysis is to select algorithms that are robust, that is to say, that do not produce a wildly different result for very small changes in the input data [19].

Definition 2.6. Consider for simplicity a uniform FD grid with spatial step h and temporal step $\Delta\tau$. A one-step FD scheme approximating a PDE is called *convergent* if for every solution to this PDE $V(x, \tau)$ at some point $x \in [0, x_{\max}]$, $t \in [0, T]$, and solutions to the FD scheme $C(x_i, \tau_n)$, $x = ih$, $\tau = \Delta\tau n$, the following hold:

- $\tau_0 = 0$, and $C(x_i, 0)$ converges to $V(x, 0)$ as ih approaches to x .
- Then $C(x_i, \tau_n)$ converges to $V(x, \tau)$ as $(ih, n\Delta\tau)$ approaches (x, t) as $h, \Delta\tau$ approach 0.

Definition 2.7. Given the PDE Eq. (2.1) and the discrete solution Eq. (2.24), the corresponding FD scheme is called *consistent* with the PDE if for every smooth function $\phi(x, \tau)$, one has

$$e^{\tau\mathcal{L}}\phi(x, \tau) - e^{\tau L}\phi(x_i, 0) \rightarrow 0,$$

as $ih \rightarrow x$, and $h \rightarrow 0$, $\Delta\tau \rightarrow 0$, where by $\phi(x_i, \tau_n)$ we understand the element of the vector of the discrete PDE solutions at the point (x_i, τ_n) .

Following [2], we regard the discrete operator $T_h = e^{\Delta\tau L}$ defined on a uniform grid $\mathbf{G}(x)$ as a linear map T_h from a vector space C_h , called the discrete solution space, to a second vector space C_h^d , called the discrete data space. We know that if the original problem for the PDE Eq. (2.1) is well posed, then by definition, the solution $V(\mathbf{x}, \tau)$ depends continuously on the initial data $V(\mathbf{x}, 0)$. On the discrete level, this continuous dependence is called *stability*. Thus, stability refers to the continuity of the map $T_h : C_h^d \rightarrow C_h$. So intuitively, an unstable discretization is one for which $|T_h|$ is very large.

Imagine that we perturb the initial data $C(\mathbf{x}, 0)$ by ϵ_h so that the initial vector is now $\tilde{C}(\mathbf{x}, 0) = C(\mathbf{x}, 0) + \epsilon_h$. This results in a perturbation of the discrete solution to $\tilde{C}(\mathbf{x}, \tau) = T_h \tilde{C}(\mathbf{x}, 0)$. Introducing the norms $\|\cdot\|_h$ in C_h^d and C_h , we obtain

$$\frac{\tilde{C}(\mathbf{x}, \tau) - C(\mathbf{x}, \tau)}{\tilde{C}(\mathbf{x}, 0) - C(\mathbf{x}, 0)} = \frac{\|T_h \epsilon_h\|_h}{\|\epsilon_h\|_h}. \quad (2.22)$$

Accordingly, the stability constant K_h is defined as the norm of the operator T_h :

$$K_h = \sup_{0 \neq \epsilon_h \in C_h^d} \frac{\|T_h \epsilon_h\|_h}{\|\epsilon_h\|_h}.$$

With these definitions in place, the error of the FD scheme can be introduced as an absolute difference

$$\begin{aligned} \epsilon &= \sup_{i \in [1, N], j \in [1, M]} \|V(x_i, \tau_n) - C(x_i, \tau_n)\|_h \\ &\leq K_h \sup_{i \in [1, N], j \in [1, M]} \|T_h^{-1} V(x_i, \tau_n) - C(x_i, 0)\|_h. \end{aligned} \quad (2.23)$$

Definition 2.8. A scheme is called *stable* if the stability constant K_h is bounded uniformly in h , i.e.,

$$K_h \leq K^{st} = \text{const}$$

for some number K^{st} and all h .

Proposition 2.1. A discretization scheme that is consistent and stable is convergent.

It can be seen that if Eq. (2.23) is applied to two consecutive time steps of an FD scheme, then the error doesn't increase if $\|T_h\|_h < 1$ regardless of the values of h and $\Delta\tau$.

Definition 2.9. The FD solution Eq. (2.24) is called unconditionally stable if $\|T_h\|_h < 1$ regardless of the values of h and $\Delta\tau$.

Since by definition, $T_h = e^{\Delta\tau L}$, the unconditional stability of T_h is given by the following proposition.

Proposition 2.2. Suppose L is a square $N \times N$ matrix. The FD scheme with transition operator $T_h = e^{\Delta\tau L}$ is unconditionally stable if in the spectral norm $\|\cdot\|_s$, we have $\|L\|_s < 0$. In other words, L has eigenvalues λ_i , $i \in [1, N]$, and $\lambda_i < 0 \forall i \in [1, N]$.

Proof. By definition, the spectral radius $\rho_s(L)$ of a matrix $L \in \mathbb{C}^{n \times n}$ is defined as [4]

$$\rho_s(L) = \max \{ |\lambda_1|, \dots, |\lambda_n| \},$$

where λ_i , $i \in [1, n]$, are the real or complex eigenvalues of L . We have

$$\| e^{\Delta\tau L} \|_s \leq e^{\|\Delta\tau L\|_s} = e^{\Delta\tau \|L\|_s} < 1.$$

The latter inequality follows because $\|L\|_s = \rho_s(L)$, and by assumption, $\rho_s(L) < 0$.

Definition 2.10. The FD solution Eq. (2.24) is called conditionally stable if $\|T_h\|_h < 1$ only when the values of h and $\Delta\tau$ satisfy some additional conditions.

It is well known that the explicit Euler scheme is only conditionally stable, while the implicit Euler and the Crank–Nicolson schemes are unconditionally stable [9]. For the latter, this can be shown using, e.g., the diffusion equation with constant diffusion coefficient D . However, the approximate solutions can still contain (decaying) spurious oscillations if $D\Delta\tau/h^2 > 1/2$ as shown by von Neumann stability analysis.

2.4.3 Nonnegativity of the Solution

For many real financial problems the solution of the corresponding PDE, given, e.g., by Eq. (2.4), should be positive, or at most nonnegative. This is the case when the solution vector is, say, the price of some instrument, for instance a stock price. Obviously, applying the operator $e^{\mathcal{L}}$ to a nonnegative vector should not result in the appearance of negative components of the vector. Small negative values, which naively can be treated as an approximation error, actually can make the whole scheme unstable, so having negative components gives rise to a situation in which the solution cannot be obtained at all. As mentioned, e.g., in the recent paper [26] in which an application of positivity-preserving schemes is considered as applied to the solution of a semilinear hyperbolic system of a correlated random walk model describing movement of animals and cells in biology, replacing a negative density or negative pressure by a positive quantity is neither a conservative cure nor a stable solution. The same is true for financial problems. Therefore, it is highly important to design a scheme that by construction preserves nonnegativity.

Before introducing a formal notion of nonnegativity of an FD scheme, note that in the continuous case, the heat equation—for example—satisfies the so-called *maximum principle*, which for an initial–boundary problem, claims that the maximum and minimum of the solution for the heat equation can be reached either at the initial moment or at the boundary of the domain; see [40] and references therein. In the discrete case, only a special class of FD schemes satisfies the discrete analogue of this principle [7], while, e.g.,

in the 2D case, the solution obtained using a nonuniform grid usually loses the maximum property. Therefore, in situations in which the maximum principle is not correct, a simpler notion of nonnegative scheme can be employed.

To define nonnegativity of a solution, we introduce the following definitions [32]. Let (M, μ) be a σ -finite measure space with μ a positive measure defined on a σ -algebra Σ of subsets of a set M (which is the countable union of measurable sets with finite measure), so $\mu(M)$ is a finite real number.

Definition 2.11. Let $f \in L^2(M, d\mu)$ be a real-valued function. Then $f(x)$ is nonnegative if $f(x) \geq 0$ μ -almost everywhere. Moreover, f is called strictly positive if $f > 0$ μ -almost everywhere.

For example, the option price $C(t, \mathbf{x})$ is a nonnegative function.

Definition 2.12. A bounded operator A on $L^2(M, d\mu)$ is said to be nonnegativity-preserving if $(f, Ag) \geq 0$ for all nonnegative $f, g \in L^2(M, d\mu)$. Such an operator A is said to be positivity-improving if $(f, Ag) > 0$ for all nonnegative $f, g \in L^2(M, d\mu)$.

Within the FD approach, the operator \mathbb{L} is discretized on a grid, which means that the function $C(t, \mathbf{x})$ is effectively replaced with a vector $C(t, \mathbf{X})$, where X is a discrete vector of prices on the grid, and the operator \mathbb{L} is replaced with a matrix L . Therefore, the formal solution Eq. (2.4) translates to

$$C(x, \tau) = e^{\tau L} C(x, 0). \quad (2.24)$$

To define a nonnegativity-preserving FD scheme, we need we need definitions similar to the above in the discrete case.

Definition 2.13. A real-valued vector $x = [x_1, \dots, x_N]$ is nonnegative if $x_i \geq 0 \ \forall i \in [1, N]$.

Definition 2.14. Given a formal solution of a linear PDE in the form of Eq. (2.24), that solution is called nonnegativity-preserving if $C(x, 0)$ is a nonnegative vector, and $C(x, \tau)$ is also a nonnegative vector.

Definition 2.15. An arbitrary matrix $A = \{a_{ij}\}$, $i \in [1, N]$, $j \in [1, M]$, is said to be nonnegative if

$$a_{ij} \geq 0, \quad \forall i, j.$$

From definitions 2.14 and 2.15, we obtain at once the following proposition.

Proposition 2.3. *The solution Eq. (2.24) is nonnegativity-preserving if $e^{\tau L}$ is a nonnegative matrix.*

Proof. The result directly follows from the definition of matrix–vector product.

A natural question now arises: what properties should a matrix L possess to guarantee that the matrix exponential $e^{\tau L}$ is a nonnegative matrix? This will be discussed in more detail in Section 3.

2.4.4 Complexity

The following definition can be found in [1].

Definition 2.16. Computational complexity is a mathematical characterization of the difficulty of a mathematical problem which describes the resources required by a computing machine to solve the problem.

The mathematical study of such characterizations is called computational complexity theory. It is important in many branches of theoretical computer science, especially cryptography. To give a practical recipe for computing complexity, the above definition can be reformulated to measure complexity as the number of steps or arithmetic operations required to solve a computational problem.

As applied to the FD schemes, the complexity is usually characterized by the number of arithmetic operations required to complete one time step $\Delta\tau$. It is well known that, e.g., the complexity of solving a system of linear equations with a dense matrix is $O(N^3)$, where N is the size of the matrix (for FD schemes, this is equal to the number of nodes on the spatial grid). Solving a system with a sparse RHS matrix can be done with a lower complexity. For instance, if one solves the Black–Scholes PDE and uses the CN scheme together with the central-order finite differences for approximation of the first and second spatial derivatives, the RHS matrix of the system of linear algebraic equations thus obtained is tridiagonal. So this system can be solved with complexity $O(N)$. Another example of reduced complexity is that of the FFT (fast Fourier transform) algorithm, which is $O(N \log N)$ [36].

Hence, complexity is an important characteristic of numerical algorithms. In this book, our goal is to construct FD schemes for solving various PDE and PIDE using the operator splitting technique, which is described in the next section and across the whole book. These schemes are designed in an attempt to achieve as much as possible that at every step of splitting, the corresponding 1D equations can be solved with linear, $O(N)$, complexity. We compare these algorithms with those existing in the literature, and explicitly mention all advantages and disadvantages of the proposed schemes, especially as compared with the FFT algorithm.

Let us underline that in practice, computing the complexity of FD scheme cannot be done exactly. Usually, the actual number of operations required for doing some numerical step can only be estimated as $T_e = \kappa N^p$, where T_e is the elapsed time, $\kappa > 0$, $p \in \mathbb{R}$, are constants. They can be retrieved, e.g., by running the same algorithm three times on grids with a different number of nodes N_1, N_2, N_3 , and then solving a system of two algebraic equations for κ and p .

2.5 Operator Splitting Technique

In the multidimensional case, to solve Eq. (2.4) we use splitting. This technique is also known as the method of fractional steps; see [10, 38, 48]. It is sometimes cited in the financial literature as Russian splitting or as locally one-dimensional schemes [9].

The method of fractional steps reduces the solution of an original k -dimensional unsteady problem to the solution of k one-dimensional unsteady equations per one full time step. For example, consider a two-dimensional diffusion equation with a solution obtained using some finite difference method. At every time step, a standard discretization in the spatial variables is applied, such that the finite difference grid contains N_1 nodes in the first dimension and N_2 nodes in the second dimension. Then the problem is to solve a system of $N_1 \times N_2$ linear equations, and the matrix of this system is block-diagonal. In contrast, the use of splitting results in, e.g., N_1 systems of N_2 linear equations, where the matrix of each system is banded (tridiagonal), is easier to implement and, more importantly, provides significantly better performance.

The described procedure uses operator splitting in different dimensions. Then this idea was further extended in [33, 42] by considering complex physical processes, e.g., diffusion in a chemically reacting gas, or the convection–diffusion problem. In addition to (or instead of) splitting in spatial coordinates, it was proposed to split a multidimensional equation into physical processes that differ in nature, e.g., convection and diffusion. This idea becomes especially efficient if the characteristic times of evolution (relaxation time) of such processes are significantly different.

2.5.1 General Approach

For a general approach to splitting techniques for *linear* operators using Lie algebras, we refer the reader to [30]. Let us again consider Eq. (2.1). Decomposing the total (compound) operator \mathcal{L} for the problem of interest seems to be natural if, say, \mathcal{L} can be represented as a sum of k commuting linear operators $\sum_{i=1}^k \mathcal{L}_i$. In this case, the formal solution of Eq. (2.1) given in Eq. (2.10) should be rewritten as

$$V(\mathbf{x}, t) = e^{t\mathcal{L}} V(\mathbf{x}, 0) = e^{t \sum_{i=1}^k \mathcal{L}_i} V(\mathbf{x}, 0). \quad (2.25)$$

Due to the commuting property, the latter expression can be factorized into a product of operators

$$V(\mathbf{x}, t) = e^{t\mathcal{L}_k} \dots e^{t\mathcal{L}_1} V(\mathbf{x}, 0).$$

This equation can then be solved in N steps sequentially by the following procedure:

$$\begin{aligned} V^{(1)}(\mathbf{x}, t) &= e^{t\mathcal{L}_1} V(\mathbf{x}, 0), \\ V^{(2)}(\mathbf{x}, t) &= e^{t\mathcal{L}_2} V^{(1)}(\mathbf{x}, t), \\ &\vdots \\ V^{(k)}(\mathbf{x}, t) &= e^{t\mathcal{L}_k} V^{(k-1)}(\mathbf{x}, t), \\ V(\mathbf{x}, t) &= V^{(k)}(\mathbf{x}, t). \end{aligned}$$

Again, this algorithm is exact (no bias) if all the operators commute.

If, however, they do not commute, the above algorithm provides only a first-order approximation in time (i.e., $O(t)$) to the exact solution. To achieve better accuracy, in the next paragraph we consider a general approach to this problem for linear equations. However, it turns out that the situation is still tractable when the whole operator \mathcal{L} is nonlinear yet can be represented as a sum of nonlinear operators \mathcal{L}_k . This case is considered briefly at the end of this section.

Linear noncommuting operators.

For noncommuting linear operators, consider the following approach [30]. Denote by $\mathcal{S}(\Delta\tau)$ the solution (semigroup) operator for Eq. (2.1), that is,

$$V(\mathbf{x}, \tau + \Delta\tau) = \mathcal{S}(\Delta\tau)V(\mathbf{x}, \tau), \quad \mathcal{S}(\Delta\tau) \equiv e^{\Delta\tau \sum_k \mathcal{L}_k},$$

and $\mathcal{S}_k(\Delta\tau) = e^{\Delta\tau \mathcal{L}_k}$ the solution operator for the subproblem

$$\frac{\partial V(\mathbf{x}, \tau)}{\partial \tau} = \mathcal{L}_k V(\mathbf{x}, \tau).$$

Let $\tilde{\mathcal{S}}_k(\Delta\tau)$ denote a consistent numerical approximation to $\mathcal{S}_k(\Delta\tau)$. For the abstract initial-boundary value problem Eq. (2.1), we may compactly represent, e.g., the celebrated Strang splitting scheme [42] by

$$\tilde{C}(\tau + \Delta\tau) = \tilde{\mathcal{S}}(\Delta\tau)C(\tau), \quad \tilde{\mathcal{S}}(\Delta\tau) = \tilde{\mathcal{S}}_1\left(\frac{1}{2}\Delta\tau\right)\tilde{\mathcal{S}}_2\left(\frac{1}{2}\Delta\tau\right)\dots \quad (2.26)$$

$$\tilde{\mathcal{J}}_{k-1} \left(\frac{1}{2} \Delta \tau \right) \tilde{\mathcal{J}}_k (\Delta \tau) \tilde{\mathcal{J}}_{k-1} \left(\frac{1}{2} \Delta \tau \right) \dots \tilde{\mathcal{J}}_2 \left(\frac{1}{2} \Delta \tau \right) \tilde{\mathcal{J}}_1 \left(\frac{1}{2} \Delta \tau \right).$$

For parabolic equations with constant coefficients, this composite algorithm is second-order accurate in $\Delta \tau$, provided that a numerical procedure that solves a corresponding equation at every splitting step is at least second-order accurate.

The solution $\tilde{C}(\tau + \Delta \tau)$ denotes the approximation to $C(\tau + \Delta \tau)$ resulting from approximately solving the subproblems $C_\tau = \mathcal{L}_k C$ in the given sequential order. The solution operator $\tilde{\mathcal{J}}$ is the resulting splitting approximation to \mathcal{J} .

Strang splitting always leads to a second-order approximation in $\Delta \tau$, at least in a formal sense. We are interested in the structure of the splitting error. Although it is tedious, local splitting errors can always be obtained by straightforward Taylor expansions. This, however, leads to an expression that does not reveal in a clear way the structure of the error. Therefore, Lanser and Verwer further adopted the Lie operator formalism. This formalism will enable us to use the celebrated Baker–Campbell–Hausdorff (BCH) formula [17]. The BCH formula yields considerable insight into the particular structure of the splitting errors.

Consider first the general differential equation (2.1) (the integral equation could be treated in the same way). With each given operator \mathcal{L} , a Lie operator is associated, which we denote by \mathcal{F} . This Lie operator is a linear operator acting on the Banach space of operators \mathbf{S} . The operator \mathcal{F} maps each operator G to a new operator $\mathcal{F}G$ such that for every element $C \in \mathbf{S}$,

$$(\mathcal{F}G)(C) = G'(C)\mathcal{L}(C),$$

where $'$ denotes differentiation with respect to C . For the solution $C(\tau)$ of Eq. (2.1), it easily follows that

$$(\mathcal{F}G)(C(\tau)) = \frac{\partial}{\partial \tau} G(C(\tau)),$$

and from induction on k that

$$(\mathcal{F}^k G)(C(\tau)) = \frac{\partial^k}{\partial \tau^k} G(C(\tau)).$$

The above relationships hold for every G defined on \mathbf{S} , in particular for the identity I . Substituting I for G and using a Taylor expansion of the true solution, we can write $C(\tau + \Delta \tau)$ in terms of the exponentiated Lie operator form or Lie–Taylor series

$$C(\tau + \Delta \tau) = (e^{\Delta \tau \mathcal{F}} I) C(\tau).$$

The same argument concerning this exponentiated Lie operator applies to each of the subproblems $C_\tau = \mathcal{L}_k C$. Hence, in composing the resulting exponentiated Lie operators

in the same order as the solution operators in the splitting procedure with which they are associated, we can reveal that the Strang splitting solution Eq. (2.26) can be expressed as

$$\begin{aligned} \tilde{C}(\tau + \Delta\tau) = & \left[e^{\frac{1}{2}\Delta\tau \mathcal{F}_1} e^{\frac{1}{2}\Delta\tau \mathcal{F}_2} \dots e^{\Delta\tau \mathcal{F}_{k-1}} \right. \\ & \left. e^{\Delta\tau \mathcal{F}_k} e^{\Delta\tau \mathcal{F}_{k-1}} \dots e^{\frac{1}{2}\Delta\tau \mathcal{F}_2} e^{\frac{1}{2}\Delta\tau \mathcal{F}_1} I \right] \tilde{C}(\tau). \end{aligned} \quad (2.27)$$

Lanser and Verwer then apply the BCH formula to say that the product $e^X e^Y$ can be written as the exponential e^Z of

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, X, Y] + [Y, Y, X]) + \frac{1}{24}[X, Y, Y, X] + \dots, \quad (2.28)$$

where $[X, Y]$ is the commutator $[X, Y] = XY - YX$, and $[X, X, Y]$ is recursively defined by $[X, X, Y] = [X, [X, Y]]$, etc. Note that if X and Y are Lie operators, then Z is also a Lie operator.

As an example, let us assume that $k = 3$. In this case, one can alternatively use the formula of Yoshida, who showed in [49] that

$$e^{tX} e^{tY} e^{tX} = e^{tZ}, \quad Z = (2X + Y) + \frac{t^2}{6}([Y, Y, X] - [X, X, Y]) + O(t^4). \quad (2.29)$$

Now put $X = \frac{1}{2}\theta \mathcal{L}_1$, etc., and apply BCH four times, or Yoshida's formula two times, which results in an expression for the symmetric Strang splitting solution,

$$\begin{aligned} \tilde{C}(\tau + \Delta\tau) = & (e^{\Delta\tau \tilde{\mathcal{F}}} I) \tilde{C}(\tau), \\ e^{\Delta\tau \tilde{\mathcal{F}}} = & e^{\frac{1}{2}\Delta\tau \mathcal{F}_1} e^{\frac{1}{2}\Delta\tau \mathcal{F}_2} e^{\Delta\tau \mathcal{F}_3} e^{\frac{1}{2}\Delta\tau \mathcal{F}_2} e^{\frac{1}{2}\Delta\tau \mathcal{F}_1}, \end{aligned} \quad (2.30)$$

where the new Lie operator $\tilde{\mathcal{F}}$ is formally defined by an infinite series expansion that is even in $\Delta\tau$. Its leading part reads

$$\begin{aligned} \tilde{\mathcal{F}} = & \mathcal{F}_1 + \mathcal{F}_2 + \mathcal{F}_3 + \frac{1}{12}\theta^2 \left\{ -2[\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3] - 2[\mathcal{F}_1, \mathcal{F}_1, \mathcal{F}_3] \right. \\ & + [\mathcal{F}_2, \mathcal{F}_2, \mathcal{F}_1] - 2[\mathcal{F}_2, \mathcal{F}_2, \mathcal{F}_3] + [\mathcal{F}_3, \mathcal{F}_3, \mathcal{F}_1] \\ & \left. + [\mathcal{F}_3, \mathcal{F}_3, \mathcal{F}_2] + [\mathcal{F}_2, \mathcal{F}_3, \mathcal{F}_1] + [\mathcal{F}_3, \mathcal{F}_2, \mathcal{F}_1] \right\} + O(\Delta\tau^4). \end{aligned} \quad (2.31)$$

To proceed, we have to be able to recover the operator $\tilde{\mathcal{L}}$ corresponding to \mathcal{L} to get the modified problem $C_\tau = \tilde{\mathcal{L}}C$ associated with the symmetric Strang splitting scheme. Lanser and Verwer show that

$$[\mathcal{F}_k, \mathcal{F}_l, \mathcal{F}_m]I(C) = \mathcal{L}'_{lm}\mathcal{L}_k - \mathcal{L}'_k\mathcal{L}_{lm}, \quad \mathcal{L}_{lm} = \mathcal{L}'_m\mathcal{L}_l - \mathcal{L}'_l\mathcal{L}_m. \quad (2.32)$$

Eventually, they rewrite this modified problem in the form

$$C_\tau = \tilde{\mathcal{L}}(C) = \mathcal{L}(C) + \tau^2 E_{\mathcal{L}}(C) + O(\tau^4), \quad (2.33)$$

where term $E_{\mathcal{L}}$ represents the leading term of the local error of the Strang splitting scheme evaluated at $C(\tau)$ and consists of various combinations of commutators of $[\mathcal{L}_k, \mathcal{L}_l, \mathcal{L}_m, \mathcal{L}_n]$.

The global error, $\tilde{C}(\tau + \Delta\tau) - C(\tau + \Delta\tau)$, can be directly seen to satisfy

$$\tilde{C}(\tau + \Delta\tau) - C(\tau + \Delta\tau) = \left(e^{\Delta\tau\tilde{\mathcal{F}}}I\right)(\tilde{C}(\tau) - C(\tau)) + \left(e^{\Delta\tau\tilde{\mathcal{F}}}I - e^{\Delta\tau\mathcal{F}}I\right)C(\tau),$$

where $\left(e^{\Delta\tau\tilde{\mathcal{F}}}I - e^{\Delta\tau\mathcal{F}}I\right)C(\tau)$ is the complete local splitting error. The local splitting error is even in τ , provided that the Lie operators are independent of τ and also even in τ .

This expression can be directly verified when all splitting operators \mathcal{L}_k commute with one another. Then $\tilde{\mathcal{L}} = \mathcal{L}$, and no splitting error occurs.

Nonlinear noncommuting operators.

For *nonlinear, noncommuting* operators, the situation is more delicate. As shown in [29], the theoretical analysis of the nonlinear initial value problem

$$u'(t) = F(u(t)), \quad 0 \leq t \leq T,$$

for a function $u : [0, T] \rightarrow X$ defined at an appropriate complex Banach space with norm $\|\cdot\|$, given an initial condition $u(0)$, could be done using the calculus of Lie derivatives. A formal linear representation of the exact solution is

$$u(t) = \mathcal{E}_F(t, u(0)) = e^{tD_F}u(0), \quad 0 \leq t \leq T,$$

where the evolution operator and Lie derivatives are given by

$$e^{tD_F}v = \mathcal{E}_F(t, v), \quad e^{tD_F}Gv = G(\mathcal{E}_F(t, v)), \quad 0 \leq t \leq T,$$

$$D_Fv = F(v), \quad D_FGv = G'(v)F(v),$$

for an unbounded nonlinear operator $G : D(G) \subset X \rightarrow X$. Using this formalism, it is shown in [29] that Strang's second-order splitting method remains unchanged in the case of nonlinear operators.

2.5.2 Splitting for a Convection–Diffusion PDE

A general analysis of the splitting technique briefly introduced in the previous section gives a powerful tool for building various splitting algorithms for FD schemes. However, e.g., the Strang scheme is not the only possible one that provides a second-order of approximation in time. Moreover, among various possible schemes, it might not be the most efficient scheme in terms of performance. Therefore, various splitting algorithms have been produced that (i) don't directly follow the general methodology, and (ii) provide the requisite order of approximation but are faster than the general scheme. Below, we give an example of such a scheme as applied to 2D and 3D convection–diffusion problems.

We follow [24], who consider the unconditional stability of second-order finite difference schemes used to solve numerically multidimensional diffusion problems containing mixed spatial derivatives. They investigate the ADI scheme proposed by Craig and Sneyd (see references in the paper), a modified version of Craig and Sneyd's ADI scheme, and the ADI scheme introduced by Hundsdorfer and Verwer. Necessary conditions are derived on the parameters of each of these schemes for unconditional stability in the presence of mixed derivative terms. The main result of [24] is that under a mild condition on the parameter θ of the scheme, the second-order Hundsdorfer and Verwer (HV) scheme is unconditionally stable when applied to semidiscretized diffusion problems with mixed derivative terms in an arbitrary spatial dimension $k > 2$.

Following [24], consider initial–boundary value problems for two-dimensional diffusion equations, which after spatial discretization lead to initial value problems for huge systems of ordinary differential equations,

$$V'(\tau) = F(\tau, V(\tau)) \quad \tau \geq 0, \quad V(0) = V_0, \quad (2.34)$$

with given vector-valued function F and initial vector V_0 . In [24], some splitting schemes for the numerical solution of Eq. (2.34) are considered. The authors assume that F is decomposed into the sum

$$F(\tau, V) = F_0(\tau, V) + F_1(\tau, V) + \cdots + F_k(\tau, V), \quad (2.35)$$

where the $k + 1$ terms $\{F_j\}$ are easier to handle than F itself. The term F_0 contains all contributions to F stemming from the mixed derivatives in the diffusion equation, and this term is always treated explicitly in the numerical time integration. Next, for each $j \geq 1$, F_j represents the contribution to F stemming from the second-order derivative in the j th spatial direction, and this term is always treated implicitly.

Further, the authors of [24] analyze two splitting schemes, and one of them is the HV scheme. This scheme defines an approximation $V_n \approx V(\tau_n)$, $n = 1, 2, 3, \dots$, by performing a series of (fractional) steps:

$$Y_0 = V_{n-1} + \Delta\tau F(\tau_{n-1}, V_{n-1}), \quad (2.36)$$

$$Y_j = Y_{j-1} + \theta\Delta\tau [F_j(\tau_n, Y_j) - F_j(\tau_{n-1}, V_{n-1})], \quad j = 1, 2, \dots, k,$$

$$\begin{aligned}
\tilde{Y}_0 &= Y_0 + \frac{1}{2}\Delta\tau [F(\tau_n, Y_k) - F(\tau_{n-1}, V_{n-1})], \\
\tilde{Y}_j &= \tilde{Y}_{j-1} + \theta\Delta\tau [F_j(\tau_n, \tilde{Y}_j) - F_j(\tau_n, Y_k)], \quad j = 1, 2, \dots, k, \\
V_n &= \tilde{Y}_k.
\end{aligned}$$

This scheme is of order two in time for every value of θ , so this parameter can be chosen to meet additional requirements.

In [24], the stability of this scheme is also investigated using von Neumann analysis. Accordingly, stability is always considered in the L_2 norm, and in order to make the analysis feasible, all coefficients in Eq. (2.36) are assumed to be constant and the boundary condition to be periodic. Under these assumptions, the matrices A_0, A_1, \dots, A_k that are obtained by finite difference discretization of the operators F_k are constant and form Kronecker products of circulant matrices.² Hence, the $\{A_k\}$ are normal and commute with each other. This implies that stability can be analyzed by considering the linear scalar ordinary differential equation

$$V'(\tau) = (\lambda_0 + \lambda_1 + \dots + \lambda_k)V(\tau), \quad (2.37)$$

where λ_j denotes an eigenvalue of the matrix A_j , $0 \leq j \leq k$. Then, by analyzing Eq. (2.37), in [24] some important theorems are proved to show unconditional stability of the splitting scheme when $\theta \geq 1/3$.

An important property of this scheme is that the mixed derivative term in the first equation of Eq. (2.36) is treated explicitly, while all further implicit steps contain only derivatives in time and one spatial coordinate. In other words, the entire 2D unsteady problem is reduced to a set of four 1D unsteady equations and two explicit equations.

For the semidiscretization of Eq. (2.36), the authors consider finite differences. All spatial derivatives are approximated using second-order central differences on a rectangular grid with constant mesh width $\Delta x_i > 0$ in the x_i -direction ($1 \leq i \leq k$). Details of this scheme implementation are discussed in [23]. The authors' experiments show that a choice of $\theta = 1/3$ for the Heston model is good. They also demonstrate that this scheme has a stiff order of convergence in time equal to 2.³

It can easily be observed that the first and third equations in Eq. (5.78) are of the same (Heston-like) type.

For the 3D problem, a similar approach is used in [16]. Although in this case, the stability analysis is more difficult, the authors observed stable solutions when they applied this scheme to solving various financial problems. We will discuss this approach in more detail in the next chapter.

²An explicit discretization of F_k in our case is discussed below.

³In other words, the order of convergence does not fluctuate significantly with time step change, and is always very close to 2.

2.A Appendix: Examples of Some HOC Schemes for Pricing American Options

We recall that an American option is an option that can be exercised at any time during its life. American options allow option holders to exercise the option at any time prior to and including its maturity date, thus increasing the value of the option to the holder relative to European options, which can be exercised only at maturity. The majority of exchange-traded options are American. For a more detailed introduction, see [8, 21].

For the sake of simplicity, consider a time-dependent Black–Scholes model for the underlying stock price S_t , so a yield curve and implied volatility term structure could be embedded into the Black–Scholes setup. Under standard assumptions [21], the Black–Scholes PDE Eq. (2.1) with the operator \mathcal{L} given in Eq. (2.2) still holds when the parameters r, r_F, q , where r_F is the forward rate, are replaced by their time-dependent counterparts $r(t), r_F(t), q(t)$. If we want to price an American put written on this stock, it is known that its price $V(S, t)$ solves the following linear complementarity problem: [22]

$$\begin{aligned} -\lambda &= \frac{\partial V}{\partial t} + \frac{\sigma^2}{2} S^2 \frac{\partial^2 V}{\partial S^2} + [r_F(t) - q(t)] S \frac{\partial V}{\partial S} - r(t) V, \\ [V - (K - S)] \lambda &= 0, \quad V - (K - S) \geq 0, \lambda \geq 0, \end{aligned} \quad (2.38)$$

subject to the terminal condition $V = \max[K - S, 0]$ and the boundary conditions

$$\begin{aligned} V &= K, \quad S = 0, \quad t \in [0, T] \\ V &\rightarrow 0, \quad S \rightarrow \infty, \quad t \in [0, T]. \end{aligned} \quad (2.39)$$

The auxiliary variable λ forces the value of the option to be higher than $K - S$.

To solve the problem Eq. (2.38) numerically, we should address some concerns, namely:

1. Equation (2.38) is not a PDE but a linear complimentary problem. So an efficient method of solving this problem has to be proposed.
2. The payoff function is not continuous in S . It is known that standard FD methods, e.g., the Crank–Nicolson method, do not preserve monotone convergence of the solution and result in error amplification or could introduce oscillations in high-frequency components of the error [28]. In other words, they change the sign of the solution, or its derivatives do so, which can cause nonphysical oscillations due to amplification in the error, depending on the relative sizes of the diffusion rate, the spatial mesh size, and time steps.
3. The first equation in Eq. (2.38) is a convection–diffusion equation. It is known that when the drift term is small compared to the diffusion term, special methods have to be used, because otherwise, the problem becomes singular (small parameter at a high-order

derivative). Usually, these methods, e.g., the exponential fitting method [9] decrease the order of the scheme. Another situation arises if one needs to correctly price deep OTM options, because for such options, Gamma is very small, while Delta is finite.

To address these issues, we proceed as follows. First, transform the original problem Eq. (2.38) into the heat equation. This is useful, since the heat equation does not contain a convection (drift) term, so it eliminates a possible singularity in the solution when the volatility is small. So by making a change of independent variables $S, t \rightarrow x, \tau$ such that

$$\tau = T - t, \quad x = \frac{1}{\sigma} \left\{ \ln S + \int_t^T \left[r_F(k) - q(k) - \frac{1}{2}\sigma^2 \right] dk \right\}, \quad (2.40)$$

we arrive to a new problem with regard to the new dependent variable $U(x, \tau)$:

$$\begin{aligned} -\lambda &= -\frac{\partial U}{\partial \tau} + \frac{1}{2} \frac{\partial^2 U}{\partial x^2} - r(\tau)U, \\ [U - (K - \xi_d e^{\sigma x})] \lambda &= 0, \quad [U - (K - \xi_d e^{\sigma x})] \geq 0, \lambda \geq 0, \\ \xi_d &\equiv \exp \left[-\int_0^\tau \left(r_r(k) - q(k) - \frac{1}{2}\sigma^2 \right) dk \right], \quad x > -\infty, \tau \in [T, 0]. \end{aligned} \quad (2.41)$$

The last step is to switch from $U(x, \tau)$ to another dependent variable $W(x, \tau)$,

$$U(x, \tau) = W(x, \tau) \xi_r, \quad \xi_r \equiv \exp \left[-\int_0^\tau r(k) dk \right], \quad (2.42)$$

which finally transforms Eq. (2.41) to the following:

$$\begin{aligned} -\lambda_1 &= -\frac{\partial W}{\partial \tau} + \frac{1}{2} \frac{\partial^2 W}{\partial x^2}, \\ [W \xi_r - (K - \xi_d e^{\sigma x})] \lambda_1 &= 0, \quad [W \xi_r - (K - \xi_d e^{\sigma x})] \geq 0, \lambda_1 \geq 0, \\ \lambda_1 &\equiv \lambda / \xi_r, \quad x > -\infty, \tau \in [T, 0]. \end{aligned} \quad (2.43)$$

The terminal condition now reads

$$W(x, 0) = \max(K - e^{\sigma x}, 0). \quad (2.44)$$

To solve this problem, a version of the operator splitting method proposed in [22] can be used. The idea is to treat the Black–Scholes operator in one fractional time step and the constraint

$$[W \xi_r - (K \xi_d - x)] \lambda_1 = 0$$

in another fractional time step. The first fractional step reads

$$-\nabla_\tau(\tilde{W}^{k+1}, W^k) + \frac{1}{2} [\theta \nabla_{x,x} \tilde{W}^{k+1} + (1 - \theta) \nabla_{x,x} W^k] + \lambda_1^k = 0, \quad (2.45)$$

where $\theta = 1$ means a fully implicit scheme, $\theta = 0$ means a fully explicit scheme, k marks the known time level, and $k + 1$ marks the unknown time level. The intermediate vector \tilde{W}^{k+1} can be efficiently solved from Eq. (2.45) using an LU decomposition.

The second fractional step enforces the constraint by projecting the solution to be feasible and updates the auxiliary variable λ_1 :

$$\begin{aligned} -\nabla_\tau(W^{k+1}, \tilde{W}^{k+1}) - \lambda_1^k + \lambda_1^{k+1} &= 0 \\ [W^{k+1} \xi_r - (K - \xi_d e^{\sigma x})] \lambda_1^{k+1} &= 0, \quad W^{k+1} \xi_r \geq (K - \xi_d e^{\sigma x}), \quad \lambda_1^{k+1} \geq 0. \end{aligned} \quad (2.46)$$

It could be checked that this method provides just a first order of approximation in time. To make it of second order, one has to choose $\theta = 1/2$ and modify the first equation in Eq. (2.46) as

$$-\nabla_\tau(W^{k+1}, \tilde{W}^{k+1}) - \frac{1}{2} (\lambda_1^k - \lambda_1^{k+1}) = 0. \quad (2.47)$$

What is important and new in our version of the method is that the implicit part of Eq. (2.45) does not depend on the option strike. The initial and boundary conditions and coefficients λ_1^k are known from the previous time level and represent an RHS of the matrix equation $A \tilde{W}^{k+1} = F(\lambda_1^k, W^k)$. Here A is a matrix that is determined by the chosen FD scheme, and F is a vector of the RHS. For instance, for the Crank–Nicolson scheme, A is a tridiagonal matrix. The fact that A does not depend on the option strike makes it possible to invert the matrix just once, and then use it for a whole bunch of strikes. These strikes vary the vector F , and therefore, a particular solution \tilde{W}^{k+1} for the strike K can be obtained by taking a product $A \cdot F(\lambda_1^k(K), W^k(K))$. This operation can be efficiently parallelized.

However, from the performance point of view it is infeasible to solve the systems with the tridiagonal matrix A in the manner described, because this algorithm is of $O(N^2)$ complexity. Instead, the well-known Thomas algorithm [20] is used, which has complexity $O(N)$. However, modification of the Thomas algorithm allows a simultaneous solution of the system with multiple RHS vectors, and this operation is very suitable for parallelizing.

It is clear that the second fractional step can be parallelized as well with the same efficiency, because for every strike computation, W^{k+1} and λ_1^{k+1} are totally independent.

2.A.1 Finite Difference Scheme

To solve Eq. (2.45) we need an FD scheme. For market making and option trading this scheme has to be highly accurate in space, fast, and stable with respect to the discontinuity in the terminal condition.

As shown by Spatz and Carey [41], for uniform grids, discretization of the heat equation of fourth order in space obtained using a compact three-point stencil reads

$$\left(1 + \frac{h^2}{12} \partial_{x,x}\right) \frac{\partial V(x, t)}{\partial t} = \partial_{x,x} V(x, t). \quad (2.48)$$

At the boundaries, we use Dirichlet boundary conditions: the option values at the boundaries are given by the Black–Scholes formula, which in our new variables reads

$$W_{call} = \frac{\xi_d}{\xi_r} e^{\sigma x + \int_0^\tau q(k) dk} N(d_1) - KN(d_2) \quad (2.49)$$

$$d_1 = \frac{x\sigma - \ln K}{\sigma \sqrt{\tau}} + \frac{3}{2} \sigma \sqrt{\tau}, \quad d_2 = \frac{x\sigma - \ln K}{\sigma \sqrt{\tau}} + \frac{1}{2} \sigma \sqrt{\tau}.$$

If $r_F = r$, the above expression changes to

$$W_{call} = e^{\sigma x + \sigma^2 \tau} N(d_1) - KN(d_2). \quad (2.50)$$

One might also want to use the Neumann boundary conditions, e.g., by specifying the option delta at the boundary.

For Eq. (2.45), the HOC schemes should be updated with a proper approximation of the source term $\lambda_1(x, \tau)$:

$$-\left(1 + \frac{h^2}{12} \partial_{x,x}\right) \frac{\partial W(x, \tau)}{\partial \tau} + \frac{1}{2} \partial_{x,x} W(x, \tau) + \left(1 + \frac{h^2}{12} \partial_{x,x}\right) \lambda_1(x, \tau) = 0. \quad (2.51)$$

In matrix notation, Eq. (2.51) reads

$$\left(I + \frac{1}{12} A_2^C\right) \frac{\partial W(x, \tau)}{\partial \tau} = \frac{1}{2h^2} A_2^C W(x, \tau) + \left(I + \frac{1}{12} A_2^C\right) \lambda_1(x, \tau) = 0. \quad (2.52)$$

For Eq. (2.45), using a backward Euler discretization in time, we obtain the following scheme:

$$\left[I + \left(\frac{1}{12} - \rho\right) A_2^C\right] W(x, \tau + \delta) = \left[I + \frac{1}{12} A_2^C\right] W(x, \tau) + \delta \left(I + \frac{1}{12} A_2^C\right) \lambda_1(x, \tau), \quad (2.53)$$

where $\rho \equiv \delta/(2h^2)$, $\delta = [T - (t + \Delta t)] - [T - t] = -\Delta t = \Delta \tau$.

The Crank–Nicolson discretization of the time derivative (which is A-stable [11]) of Eq. (2.51) reads

$$\begin{aligned} \left[I + \left(\frac{1}{12} - \frac{\rho}{2} \right) A_2^C \right] W(x, \tau + \delta) &= \left[I + \left(\frac{1}{12} + \frac{\rho}{2} \right) A_2^C \right] W(x, \tau) \\ &+ \frac{3\delta}{2} \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau) - \frac{\delta}{2} \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau - \delta). \end{aligned} \quad (2.54)$$

However, one has to remember that we do not just solve Eq. (2.51) but use a two-step splitting scheme. Therefore, to provide the total second order of approximation of the source term at the first step, one has to use a different scheme, which is

$$\begin{aligned} \left[I + \left(\frac{1}{12} - \frac{\rho}{2} \right) A_2^C \right] W(x, \tau + \delta) &= \\ \left[I + \left(\frac{1}{12} + \frac{\rho}{2} \right) A_2^C \right] W(x, \tau) &+ \delta \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau). \end{aligned} \quad (2.55)$$

The backward differentiation formula (BDF2) [22] is second-order accurate in time and also A-stable. However, it is known that this scheme better damps oscillations in the solution corresponding to high wave numbers in the Fourier expansion of the solution. Using BDF2 for Eq. (2.45), we obtain

$$\begin{aligned} \left[I + \left(\frac{1}{12} - \frac{\rho}{3} \right) A_2^C \right] W(x, \tau + \delta) &= \left(I + \frac{1}{12} A_2^C \right) \left[\frac{4}{3} W(x, \tau) - \frac{1}{3} W(x, \tau - \delta) \right] \\ &+ \frac{2\delta}{3} \left[2 \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau) - \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau - \delta) \right]. \end{aligned} \quad (2.56)$$

Again, for this splitting method the first step should be modified to read

$$\begin{aligned} \left[I + \left(\frac{1}{12} - \frac{\rho}{3} \right) A_2^C \right] W(x, \tau + \delta) &= \left(I + \frac{1}{12} A_2^C \right) \left[\frac{4}{3} W(x, \tau) - \frac{1}{3} W(x, \tau - \delta) \right] \\ &+ \delta \left(I + \frac{1}{12} A_2^C \right) \lambda_1(x, \tau). \end{aligned} \quad (2.57)$$

These versions of the CN and BDF2 schemes have a total accuracy of $O(\tau^2 + \tau^2 h^2 + h^4)$.

2.A.2 Higher-Order FD Schemes in Time

It is known that high-order finite difference schemes in time as applied to the diffusion equation not only provide better accuracy but also have better damping properties in case of nonuniform initial data. Therefore, it is reasonable to build a scheme that could be at least $O(h^4 + \delta^4)$. One family of such algorithms utilizes diagonal Padé schemes combined with positivity-preserving Padé schemes as damping devices [50]. However, these schemes

are of second order in space, and making them of higher order in space introduces an unreasonable extra complexity. Therefore, we will use a different approach [6], which we have modified accordingly for our problem.

In [6], the authors describe a one-parameter family of unconditionally stable third-order time-integration schemes, based on the extended trapezoid rules. They show that among them there exists an unconditionally L-stable method that is of third order and reads (where for the sake of brevity we use the notation $A \equiv A_2^C$)

$$\begin{aligned} \left(I - \frac{2}{3}\rho A + \frac{1}{6}\rho^2 A^2\right) W(x, \tau + \delta) &= \left(I + \frac{1}{3}\rho A\right) W(x, \tau) \\ &+ \frac{\rho}{6} [c(\tau) + 4c(\tau + \delta/2) + c(\tau + \delta)] \\ c(\tau) &\equiv [a(\tau), 0 \dots 0, b(\tau)]^T, \end{aligned} \quad (2.58)$$

and $a(t), b(t)$ are the lower and upper boundary conditions. The matrix on the left-hand side of Eq. (2.58) is pentadiagonal. This method provides an accuracy of $O(h^2 + \delta h^2 + \delta^3)$. For our purposes, we need to modify it, taking into account that we need a fourth-order approximation in space, and also that we have a source term on the right-hand side of Eq. (2.51). The source term can be taken into account using the same extended trapezoid rule (see [6]). Omitting some tedious algebra, we obtain instead of Eq. (2.58),

$$\begin{aligned} \left(I - \frac{2}{3}\rho A + \frac{1}{6}\rho^2 A^2\right) W(x, \tau + \delta) &= \left(I + \frac{1}{3}\rho A\right) W(x, \tau) \\ &+ \frac{\rho}{6} [c(\tau) + 4c(\tau + \delta/2) + c(\tau + \delta)] + \frac{\delta}{6} [6\lambda_1(x, \tau) - \delta\rho A\lambda_1(x, \tau - \delta)] . \end{aligned} \quad (2.59)$$

To modify this scheme to be of fourth order in space, we have to rewrite Eq. (2.52) in the form

$$\begin{aligned} \frac{\partial W(x, \tau)}{\partial \tau} &= \frac{1}{2h^2} \bar{A} W(x, \tau) + \lambda_1(x, \tau) = 0 \\ \bar{A} &\equiv \left(I + \frac{1}{12}A\right)^{-1} A \end{aligned} \quad (2.60)$$

and substitute the operator A with the operator \bar{A} in Eq. (2.59), which gives

$$\begin{aligned} \left[D^2 - \frac{2}{3}\rho D A + \frac{1}{6}\rho^2 A^2\right] \bar{W}(x, \tau + \delta) &= \left[D^2 + \frac{1}{3}\rho D A\right] W(x, \tau) \\ &+ \frac{\rho}{6} [c(\tau) + 4c(\tau + \delta/2) + c(\tau + \delta)] D^2 + \frac{\delta}{6} [6D^2\lambda_1(x, \tau) - \rho D A\lambda_1(x, \tau - \delta)] , \\ D &\equiv \left(I + \frac{1}{12}A\right) . \end{aligned} \quad (2.61)$$

The second step of the splitting method now has to be slightly modified to provide the total third order of accuracy in time, namely

$$\begin{aligned}
 -W(x, \tau + \delta) + \bar{W}(x, \tau + \delta) &= \frac{\delta}{12} [4\lambda_1(x, \tau) + \lambda_1(x, \tau - \delta) - 5\lambda_1(x, \tau + \delta)] \quad (2.62) \\
 [W(x, \tau + \delta)\xi_r - (K - \xi_d e^{\sigma x})] \lambda_1^{k+1} &= 0, \quad W(x, \tau + \delta)\xi_r \geq (K - \xi_d e^{\sigma x}), \\
 \lambda_1^{k+1} &\geq 0.
 \end{aligned}$$

2.A.3 L-Stable Scheme of Fifth Order in Time

Another method also proposed in [6] uses an extended Simpson rule to integrate the diffusion equation in time. The original scheme reads

$$\begin{aligned}
 \left[I - \frac{3}{5}\rho A + \frac{3}{20}\rho^2 A^2 - \frac{1}{60}\rho^3 A^3 \right] W(x, \tau + \delta) &= \left[I + \frac{2}{5}\rho A + \frac{1}{20}\rho^2 A^2 \right] W(x, \tau) \\
 &+ \frac{1}{12} \left(I + \frac{2}{5}\rho A \right) c(\tau) + \frac{1}{3} \left(I - \frac{1}{10}\rho A \right) c(\tau + \delta/2) \\
 &+ \frac{1}{12} \left(I - \frac{3}{5}\rho A + \frac{1}{10}\rho^2 A^2 \right) c(\tau + \delta). \quad (2.63)
 \end{aligned}$$

More interestingly, the septadiagonal coefficient matrix of the scheme Eq. (2.63)) can be further factorized, providing

$$\begin{aligned}
 I - \frac{3}{5}\rho A + \frac{3}{20}\rho^2 A^2 - \frac{1}{60}\rho^3 A^3 \quad (2.64) \\
 = \left\{ I - \frac{1}{30}(6 + 3s - s^2)\rho A \right\} \left\{ I - \frac{1}{30}(12 - 3s + s^2)\rho A - \frac{1}{120}(3 - s + s^2)\rho^2 A^2 \right\},
 \end{aligned}$$

where $s = 3^{1/3}$. Thus, for the scheme Eq. (2.63)) we need to solve a tridiagonal and a pentadiagonal linear system at every time step of integration. The advantage of the above scheme is that it is unconditionally L-stable and has a fifth order of approximation in time.

Now following the same idea, for the American option pricing problem we first add a source term to this scheme to obtain

$$\begin{aligned}
 \left[I - \frac{3}{5}\rho A + \frac{3}{20}\rho^2 A^2 - \frac{1}{60}\rho^3 A^3 \right] W(x, \tau + \delta) &= \left[I + \frac{2}{5}\rho A + \frac{1}{20}\rho^2 A^2 \right] W(x, \tau) \\
 &+ \frac{1}{12} \left(I + \frac{2}{5}\rho A \right) c(\tau) + \frac{1}{3} \left(I - \frac{1}{10}\rho A \right) c(\tau + \delta/2) \quad (2.65) \\
 &+ \frac{1}{12} \left(I - \frac{3}{5}\rho A + \frac{1}{10}\rho^2 A^2 \right) c(\tau + \delta) - \frac{\delta}{60} \left\{ 2(5I + 2\rho A)\lambda(x, \tau) \right. \\
 &\left. + 4(10I - \rho A)\lambda(x, \tau + \delta/2) + (10I - 6\rho A + \rho^2 A^2)\lambda(x, \tau + \delta) \right\}.
 \end{aligned}$$

Now using the same substitution as in Eq. (2.60), we obtain the final representation of the L-stable scheme with accuracy $O(\delta^5 + \delta h^4 + h^4)$:

$$a_1 a_2 W(x, \tau + \delta) = a_3 W(x, \tau) + c_1 c(\tau) + c_2 c(\tau + \delta/2) + c_3 c(\tau + \delta) \quad (2.66)$$

$$- \frac{\delta}{60} \left\{ d_1 \lambda(x, \tau) + d_2 \lambda(x, \tau + \delta/2) + d_3 \lambda(x, \tau + \delta) \right\},$$

where

$$a_1 = I + \left[\frac{1}{12} - \frac{1}{30}(6 + 3s - s^2)\rho \right] A, \quad (2.67)$$

$$a_2 = (I + \frac{1}{12}A)^2 - \frac{1}{30}(12 - 3s + s^2)(I + \frac{1}{12}A)\rho A - \frac{1}{120}(3 - s + s^2)\rho^2 A^2,$$

$$a_3 = (I + \frac{1}{12}A) \left[(I + \frac{1}{12}A)^2 + \frac{2}{5}(I + \frac{1}{12}A)\rho A + \frac{1}{20}\rho^2 A^2 \right],$$

$$c_1 = (I + \frac{1}{12}A)^2 \frac{1}{12} \left[I + (\frac{1}{12} + \frac{2}{5}\rho)A \right],$$

$$c_2 = (I + \frac{1}{12}A)^2 \frac{1}{3} \left[I + (\frac{1}{12} - \frac{1}{10}\rho)A \right],$$

$$c_3 = (I + \frac{1}{12}A) \frac{1}{12} \left[(I + \frac{1}{12}A)^2 - \frac{3}{5}(I + \frac{1}{12}A)\rho A + \frac{1}{10}\rho^2 A^2 \right],$$

$$d_1 = 2(I + \frac{1}{12}A)^2 \left[5I + (\frac{5}{12} + 2\rho)A \right],$$

$$d_2 = 4(I + \frac{1}{12}A)^2 \left[10I + (\frac{5}{6} - \rho)A \right],$$

$$d_3 = (I + \frac{1}{12}A) \left[10(I + \frac{1}{12}A)^2 - 6\rho(I + \frac{1}{12}A)A + \rho^2 A^2 \right].$$

Certainly, the second step of the splitting method has to be adjusted accordingly to provide the fifth order of accuracy in time.

One problem with this scheme is that it uses values of $\lambda_1(x, \tau + \delta/2)$ that do not belong to the grid nodes. So they could be found by interpolation. However, this interpolation must provide the fourth order of accuracy in order not to break the total accuracy of the scheme.

2.A.4 Boundary Conditions for a High-Order Uniform FD Scheme

Applied to the HOC scheme Eq. (2.58), the standard Dirichlet boundary conditions need to be consistent with the accuracy of the FD scheme. To achieve this, we use the following

algorithm. If a pentadiagonal system of linear equations has to be solved, we need to provide ghost points at which the option value should be determined by the appropriate boundary conditions. As these points we use $x_{-1} = x_{\min} - h$, $x_{-2} = x_{\min} - 2h$ at the left boundary, and $x_{N+1} = x_{\max} + h$, $x_{N+2} = x_{\max} + 2h$ at the right boundary of the grid. We assume that at all ghost points, the boundary conditions are given by the Black–Scholes formula.

Next, in Eq. (2.61) we define matrices M_1 and M_2 as

$$M_1 = D^2 - \frac{2}{3}\rho DA + \frac{1}{6}\rho^2 A^2, \quad M_2 = D^2 + \frac{1}{3}\rho DA,$$

which are completely symmetric by the assignment

$$\begin{aligned} M_1(1, 1) &= M_1(2, 2), & M_1(N, N) &= M_1(N-1, N-1) \\ M_2(1, 1) &= M_2(2, 2), & M_2(N, N) &= M_2(N-1, N-1). \end{aligned} \quad (2.68)$$

After that, on the right-hand side of Eq. (2.61), we compute the product $R = M_2 W(x, \tau)$ and modify it using the following correction terms:

$$\begin{aligned} R(1) &= R(1) + M_2(3, 1)BC(x_{-2}, t) + M_2(2, 1)BC(x_{-1}, t) \\ &\quad - (M_1(3, 1)BC(x_{-2}, t + \delta) + M_1(2, 1)BC(x_{-1}, t + \delta)) \\ R(2) &= R(2) + M_2(3, 1)BC(x_{-1}, t) - M_1(3, 1)BC(x_{-1}, t + \delta) \\ R(N-1) &= R(N-1) + M_2(1, 3)BC(x_{N+1}, t) - M_1(1, 3)BC(x_{N+1}, t + \delta) \\ R(N) &= R(N) + M_2(1, 2)BC(x_{N+1}, t) + M_2(1, 3)BC(x_{N+2}, t) \\ &\quad - (M_1(1, 2)BC(x_{N+1}, t + \delta) + M_1(1, 3)BC(x_{N+2}, t + \delta)), \end{aligned} \quad (2.69)$$

where $BC(x, t)$ denotes the boundary condition taken at the point (x, t) .

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