An Euler-Maruyama Method for Diffusion Equations with Discontinuous Coefficients and a Family of Interface Conditions

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Abstract

Numerical methods are developed for linear parabolic equations in one spatial dimension having piecewise constant diffusion coefficients along with a one parameter family of interface conditions at the discontinuity. We construct an Euler-Maruyama numerical method for the stochastic differential equation (SDE) corresponding to the alternative divergence formulation of these equations. Our main result is the construction of an Euler scheme that can accommodate specification of any one of a family of interface conditions considered. We then prove convergence estimates for the Euler scheme. To illustrate our method and its theoretical analysis we implement it for the stochastic formulation of the parabolic system.

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1. Introduction

The computational simulation of solutions to linear parabolic partial differential equations (PDEs) requires the use of highly efficient numerical methods which are consistent, stable, and potentially have high orders of accuracy.

Diffusion equations provide one of the standard approaches to modeling population dynamics with dispersal in spatially patchy environments [1, 2]. In diffusion models, the transmission properties at interfaces may be coupled to physically discrete, discontinuous properties of the environment such as river networks [3] or landscape topography and meteorological conditions [4, 5, 6, 7, 8].

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There are a number of empirical studies that indicate that the dispersal behavior of individuals, such as species of insects including aphids, beetles and caterpillar, foraging honey bees as well as several species of butterflies, is influenced by boundaries (interfaces) between different types of habitats (patches) [9, 10, 11, 12]. The survey paper ([13]) also highlights examples of dispersion in the presence of a discontinuous interface, with applications in such disparate areas as hydrology, ecology, finance, astrophysics and physical oceanography.

In recent work on interfacial effects [14, 15, 16], the authors analyze the underlying stochastic process determined by the diffusion equation in divergence form and having a specific interfacial condition in the presence of discontinuities in diffusion coefficients across interfaces. The theory of Brownian motion applies to diffusion models in homogeneous media with constant coefficients [17]. However, the discontinuity in the diffusion tensor at the interface between two media 'skews' the basic particle motion. Incorporating bias in behavior/movement at an interface or patch boundary into diffusion models naturally leads to *Skew Brownian Motion (SBM)* [18, 19, 20, 21] at the mathematical foundations, from which the underlying stochastic particle motions across the discontinuity, called α-skew diffusion, can be constructed [14]. SBM assumes that particles (individuals) move according to ordinary diffusion until they encounter an interface, but at an interface the probability that a particle (individual) will move into the region on one side of the interface is different than the chance that it will move into the region on the opposite side.

In [15, 16, 21] a conservative interface condition requiring continuity of flux is analyzed. In [14, 22], a one parameter family of interface conditions is considered, and the effects of this family of interfacial discontinuities in the diffusion coefficient on natural modifications of certain basic functionals of the diffusion, such as local time and occupation times, is analyzed. These results extend previous work in [15, 16] for conservative interface conditions and their effect on first passage times. The main goal in [14, 22] was to obtain a characterization of parameters and behavior at the macroscopic scale in terms of underlying stochastic particle motions. To achieve this goal, an equivalent formulation of the diffusion problem in terms of solutions to stochastic differential equations (SDEs) was considered. The effect of the interface was incorporated in an added drift rate involving the local time [15, 22] of the process (the stochastic counterpart of the interface condition). In particular it was shown that, at the volumetric scale of particle concentrations, the continuity of flux at an interface can be viewed as continuity of natural local time on the stochastic particle scale. As discussed at length in [22], unlike the case of homogeneous diffusion, i.e., standard Brownian motion, physical modeling in this context requires a specific choice of *local time* from among the possible variants in the literature, namely: semimartingale local time, diffusion local time, and/or natural local time. While the relationship between these various notions of local time can readily be derived, the selection of natural local time is based on the physically desirable condition of continuity of flux.

The numerical simulation of SDEs is a very active research area that has been witness to substantial progress [23, 24]. In particular, the numerical simulation of SDEs corresponding to divergence form operators involving a discontinuous coefficient has been the subject of various articles in the recent past. In the one dimensional (spatial) context, schemes based on random walks [25, 26, 27, 28], Euler methods and stochastic Taylor expansions [29, 30], and exact simulation methods [31, 32, 33, 34] have been developed for the approximation of the solution of SDEs corresponding to conservative interface conditions (and consequently self-adjoint interface conditions). In [35], the authors apply benchmark tests to four schemes with constant time steps and demonstrate the accurate or odd behavior of each scheme when computing the steady state and the transient regime.

In a closely related area, that of numerical methods for SDEs with irregular coefficients, there has also been a lot of progress. In [36], the authors analyze an Euler method in the case of non-regular drift. In [37], an Euler scheme is designed that converges weakly to the solution if the diffusion coefficient is discontinuous. However, to prove convergence and obtain the rate of convergence, Hölder continuity is required. Strong approximation of an Euler-Maruyama scheme is considered in [38], but a low convergence rate of $O(1/\log n)$ is obtained. In [39], an Euler algorithm for SDEs with discontinuous diffusion coefficients depending only on time is designed and convergence is proved. Thus, while a variety of approximations to SDEs with discontinuous diffusion coefficients exist, the *types* of convergence, and *convergence rates* continue to require refinements of existing computational techniques.

In this paper, we consider the numerical discretization of diffusion equations with discontinuous diffusion coefficients associated to a one parameter family of interface conditions. The key idea that we employ is a change of variables that transforms the given diffusion problem with the one parameter family of interface conditions into one that involves a natural continuity of flux interface condition. This change of variables is a form of *symmetrization* that renders the problem into a self-adjoint formulation. The symmetrization will help us to deal with more general specifications of interface conditions (than the conservative case), and can be used in either a deterministic or stochastic numerical framework. In this paper, we pursue the stochastic numerical approach. As done in [14], we consider in this paper an equivalent formulation of the discontinuous diffusion problem in terms of solutions to specific SDEs. The main contribution of this paper is the construction and analysis of an Euler-Maruyama numerical method to discretize these SDEs [40], following the approach developed by Martinez and Talay in [30]. Whereas these authors considered parabolic equations with discontinuous coefficients, requiring solutions with discontinuous first derivatives, the interface conditions adopted in their work makes the product of the diffusion coefficient and the first derivative of the solution a continuous function throughout the domain under consideration. In this paper, motivated by different applications, we are naturally lead to consider more general problems in which the product of the derivative of the solution and the diffusion coefficient remains discontinuous. This generality requires a more careful study of the error estimates in the Euler-Maruyama method at the interface than the one required in [30].

The paper is organized as follows. We first introduce a natural one parameter family of possible interface conditions coupled to a diffusion problem, with discontinuous diffusion coefficient, in one spatial dimension (Section 2). Motivating areas of application from the engineering, ecological and biological sciences are briefly noted. We then present a reformulation (symmetrization) of this problem which naturally can allow the application of deterministic numerical methods. Next, we introduce the corresponding stochastic differential equation formulation in Section 2.1. In Section 3 we develop an Euler-Maruyama scheme for numerically discretizing the SDE formulation that is applicable to any one of the interface conditions under consideration. In Section 4 we prove convergence of the Euler-Maruyama scheme under mild assumptions following the general approach of Martinez and Talay [30], adapted to deal with the more general interface conditions considered in this paper. Finally, numerical simulations are provided that illustrate our theoretical results and also provide comparison with other approaches to solve the discontinuous diffusion problem in Section 5.

2. Diffusion with Discontinuous Coefficients

We consider the time dependent diffusion equation in one dimension with a piecewise discontinuous diffusion coefficient across an interface at $x = 0$ on which a one parameter family of interface conditions is prescribed. We define the time interval $J = [0, T]$ and the domain $\Omega = \mathbb{R}$. The corresponding initial value problem on $\Omega \times J$ is given as

$$\frac{\partial u}{\partial t}(t,x) = \frac{\partial}{\partial x}\left(\frac{D(x)}{2}\frac{\partial u(t,x)}{\partial x}\right), \quad \forall x \in \Omega\backslash\{0\},\ t \in J \setminus \{0\}, \tag{2.1a}$$

$$u(t,0^+) = u(t,0^-), \forall\, t \in J, \tag{2.1b}$$

$$\lambda\frac{\partial u}{\partial x}(t,0^+) = (1-\lambda)\frac{\partial u}{\partial x}(t,0^-),\ \forall\, t \in J, \tag{2.1c}$$

$$u(0,x) = u_0(x), \forall\, x \in \Omega. \tag{2.1d}$$

In model (2.1) the diffusion coefficient D is piecewise defined by

$$D(x) = \begin{cases} D^+ & \text{if } x > 0, \\ D^- & \text{if } x < 0, \end{cases} \tag{2.2}$$

for some positive constants D^+, D^-. We assume initial data $u(0,x) = u_0(x)$ given for all $x \in \Omega$ in equation (2.1d). Continuity of the solution $u(t,x)$ at the interface $x = 0$ given in (2.1b), as well as a condition at $x = 0$ given in (2.1c) that depends on a parameter λ with $0 < \lambda < 1$, and involves the derivative of the solution, specify the nature of the interface. The choice of the value of λ varies according to the application, and may be a function of D^+ and D^-.

Remark 1. *One may note that the extreme cases in which $\lambda = 0, 1$, respectively, correspond to Neumann boundary conditions at the point of interface. In* *particular, therefore the coefficients are purely constant (smooth) on the corresponding half-line and amenable to standard approaches to Neumann boundary value problems. From this perspective there is no loss to restricting considerations to* $0 < \lambda < 1$.

From the point of view of applications to environmental sciences, the cases of $\lambda = \lambda^* := \dfrac{D^+}{D^+ + D^-}$ (continuity of flux), $\lambda = \lambda^\# := 1/2$ (continuity of derivatives), and $\lambda = 0$, arise as solute transport interfaces [14, 41, 22], upwelling of ocean current modeling [42], and one-sided barrier (reflective) regions, respectively. There are ecological species, example Fender's blue butterfly, and aphids for which inter-facial effects are widely reported from experiments, but the precise interface condition is unknown from a mathematical perspective, e.g., see [9, 10]. For the latter, the problem of determining λ can also be treated as a statistical problem.

Remark 2. *In order to formulate the problem for easy application of numerical methods, especially deterministic schemes, it is convenient to relate the parameter* λ *in the interface condition* (2.1c) *to one which appears in a reformulation of problem* (2.1) *written in self-adjoint form. We do this via multiplication of both sides of the PDE in* (2.1a) *by a piecewise defined (positive) function*

$$c(x) = \begin{cases} c^+ := \lambda/D^+ & \text{if } x > 0, \\ c^- := (1-\lambda)/D^- & \text{if } x < 0. \end{cases} \tag{2.3}$$

The resulting PDE can be written

$$c(x)\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u}{\partial x}\right), \quad \forall x \in \Omega\backslash\{0\}, t \in J \setminus \{0\}, \tag{2.4}$$

where the positive function κ *is defined as*

$$\kappa(x) = c(x)\frac{D(x)}{2} = \begin{cases} \kappa^+ := \frac{\lambda}{2} & \text{if } x > 0, \\ \kappa^- := \frac{(1-\lambda)}{2} & \text{if } x < 0. \end{cases} \tag{2.5}$$

Thus, the interface condition (2.1c) *may be interpreted as*

$$\left[\kappa\frac{\partial u}{\partial x}\right] := \kappa^+\frac{\partial u}{\partial x}(t, 0^+) - \kappa^-\frac{\partial u}{\partial x}(t, 0^-) = 0, \tag{2.6}$$

i.e., the jump *across the interface of* $\kappa\frac{\partial u}{\partial x}$ *at* $x = 0$*, denoted as*$\left[\kappa\frac{\partial u}{\partial x}\right]$*, is zero. Thus, problem* (2.1) *can be reformulated to have an interface condition that resembles a natural flux condition (conservative) which is more easily amenable to numerical discretization. The reformulated version of problem* (2.1) *on* $\Omega = \mathbb{R}$

can be stated as

$$c(x)\frac{\partial u}{\partial t}(t,x) = \frac{\partial}{\partial x}\left(\kappa(x)\frac{\partial u(t,x)}{\partial x}\right), \quad \forall x \in \Omega\backslash\{0\},\ t \in J \setminus \{0\}, \tag{2.7a}$$

$$[u] := u(t,0^+) - u(t,0^-) = 0,\ \forall\ t \in J, \tag{2.7b}$$

$$\left[\kappa\frac{\partial u}{\partial x}\right] := \kappa^+\frac{\partial u}{\partial x}(t,0^+) - \kappa^-\frac{\partial u}{\partial x}(t,0^-) = 0,\ \forall\ t \in J, \tag{2.7c}$$

$$u(0,x) = u_0(x), \forall x \in \Omega. \tag{2.7d}$$

We note that c plays the role of specific heat capacity times mass density of the material, and κ is a thermal conductivity, in the context of heat flow. We observe that for the special case of $\lambda = \lambda^* := D^+/(D^+ + D^-)$ we have that $c(x) \equiv \text{constant}$.

2.1. Stochastic Representation of the Solution

In this section, it will be shown that stochastic representations of solution $u(t,x)$ to (2.1) can be obtained by the analysis of stochastic differential equations with piecewise constant coefficients driven by a Brownian motion and the local time. We can also use probability techniques to derive pointwise estimates for partial derivatives of this solution.

Let us first record a definition of skew Brownian motion $B^{(\alpha)}(t)$, $0 < \alpha < 1$, originally introduced by Itô and McKean. Let $|B(t)|$ denote the reflecting Brownian motion starting at 0 defined on a complete probability space $(\Omega, \mathcal{F}, \mathbb{P})$, and enumerate the excursion intervals away from 0 by $J_1, J_2, \ldots$. Let $A_1, A_2, \ldots$ be an independent identically distributed sequence of Bernoulli ± 1 random variables, independent of $B(t)$, with $\mathbb{P}(A_n = 1) = \alpha$. Then $B^{(\alpha)}(t)$ is defined by changing the signs of the excursion over the intervals J_n whenever to $A_n = -1$, for $n = 1, 2, \ldots$. That is,

$$B^{(\alpha)}(t) = \sum_{n=1}^{\infty} A_n \mathbf{1}_{J_n}(t)|B(t)|, \quad t \geq 0. \tag{2.8}$$

For $x \in \mathbb{R}$ and $t \geq 0$ denote $\sigma(x) = \sqrt{D^+}x\mathbf{1}_{[0,\infty)}(x) + \sqrt{D^-}x\mathbf{1}_{(-\infty,0)}(x)$ and

$$Y^{(\alpha)}(t) = \sigma\big(B^{(\alpha)}(t)\big). \tag{2.9}$$

For each $g \in C_b^2(\mathbb{R} \setminus \{0\})$ and $x \neq 0$ we denote the operator

$$\tilde{\mathcal{L}}g(x) = \frac{D(x)}{2}g''(x). \tag{2.10}$$

In addition, denote the functional spaces

$$\begin{aligned}\mathcal{W}^2 = \Big\{ & g \in C_b^2\big(\mathbb{R}\setminus\{0\}\big) : g^{(i)} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}), i = 1,2; \\ & \lambda g'(0^+) = (1-\lambda) g'(0^-),\ g''(0^+) = g''(0^-) \Big\}, \end{aligned} \tag{2.11}$$

$$\begin{aligned}\mathcal{W}^4 = \Big\{ & g \in C_b^4\big(\mathbb{R}\setminus\{0\}\big) : g^{(i)} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}), i = 1,\dots,4; \\ & \lambda g'(0^+) = (1-\lambda) g'(0^-),\ g''(0^+) = g''(0^-), \\ & \lambda(\tilde{\mathcal{L}}g)'(0^+) = (1-\lambda)(\tilde{\mathcal{L}}g)'(0^-),\ (\tilde{\mathcal{L}}g)''(0^+) = (\tilde{\mathcal{L}}g)''(0^-) \Big\}. \end{aligned} \tag{2.12}$$

Note that any function in $\mathcal{W}^2$ or $\mathcal{W}^4$ can be written as a difference of two convex functions. Now we are in a position to state the stochastic representation theorem which can be found in [41] (see also [30]).

Theorem 3 (Corollary 2.2 from [41]). *Let $0 < \lambda < 1$, $u_0 \in \mathcal{W}^2$, and*

$$\alpha = \alpha(\lambda) = \frac{\lambda\sqrt{D^-}}{\lambda\sqrt{D^-} + (1-\lambda)\sqrt{D^+}}. \tag{2.13}$$

Then the function

$$u(t,x) = \mathbb{E}^x u_0(Y^{(\alpha)}(t)), \quad (t,x) \in [0,T] \times \mathbb{R} \tag{2.14}$$

is the unique function in $C_b^{1,2}([0,T] \times (\mathbb{R}\setminus\{0\})) \cap C([0,T]\times\mathbb{R})$ which satisfies the equations (2.1).

It follows from the proof of [41, Theorem 2.1] that if $f \in C^2(\mathbb{R}\setminus\{0\}) \cap C(\mathbb{R})$ satisfying the conditions $\lambda f'(0^+) = (1-\lambda) f'(0^-)$ and $f''(0^+) = f''(0^-)$ then, for $\alpha = \alpha(\lambda)$ as in (2.13), we have

$$\begin{aligned} f\big(Y^{(\alpha)}(t)\big) = f\big(Y^{(\alpha)}(0)\big) &+ \int_0^t f'_-\big(Y^{(\alpha)}(s)\big)\sqrt{D\big(Y^{(\alpha)}(s)\big)}dB(s) \\ &+ \frac{1}{2}\int_0^t D\big(Y^{(\alpha)}(s)\big) f''\big(Y^{(\alpha)}(s)\big)ds, \end{aligned} \tag{2.15}$$

where $f'_-(x)$ denotes one sided left derivative and $f''(x)$ is the usual second derivative for $x \neq 0$. In fact, (2.15) is the first equation on page 389 in [41] with the term relating to the local time equaling 0. In addition, $Y^{(\alpha)}(t)$ satisfies the following stochastic differential equation with a local time

$$dY^{(\alpha)}(t) = \sqrt{D\big(Y^{(\alpha)}(t)\big)}dB(t) + \left(\frac{\sqrt{D^+} - \sqrt{D^-}}{2} + \sqrt{D^-}\frac{2\alpha - 1}{2\alpha}\right) dl_t^{B^{(\alpha)},+}(0) \tag{2.16}$$

where $D(x)$ is defined as in (2.2), the local time $l_t^{B^{(\alpha)},+}(0)$ is defined by

$$l_t^{B^{(\alpha)},+}(0) = \lim_{\epsilon \downarrow 0} \frac{1}{\epsilon}\int_0^t \mathbf{1}_{[0,\epsilon)}(B^{(\alpha)}(s)) d\langle B^{(\alpha)}\rangle_s,$$

and $\langle B^{(\alpha)}\rangle_s$ denotes the quadratic variation of $B^{(\alpha)}(s)$.

Next, we have some pointwise estimates for the derivatives of $u(t,x)$. A similar result for the case of $\lambda = \frac{D^+}{D^+ + D^-}$ (continuity of flux) was given in [30].

Theorem 4. *Let $0 < \lambda < 1$, $\alpha = \alpha(\lambda)$ as in* (2.13)*, and $Y^{(\alpha)}(t)$ the solution of the SDE* (2.16)*.*

Part I: The probability distribution of $Y^{(\alpha)}(t)$ under $\mathbb{P}^x$ (i.e. $Y^{(\alpha)}(0) = x$) has a density $q^{(\alpha)}(t,x,y)$ continuous for $t > 0$, $x \in \mathbb{R}$, and $y \in \mathbb{R} \setminus \{0\}$. Furthermore, there exists a constant $C > 0$ such that for all $x \in \mathbb{R}$, $t > 0$, and $y \in \mathbb{R} \setminus \{0\}$,

$$q^{(\alpha)}(t,x,y) \leq \frac{C}{\sqrt{t}}, \tag{2.17}$$

and such that for all $x \in \mathbb{R}$, $t > 0$, and $u_0 \in L^1(\mathbb{R})$,

$$\left| \mathbb{E}^x u_0\big(Y^{(\alpha)}(t)\big) \right| \leq \frac{C}{\sqrt{t}} \|u_0\|_1. \tag{2.18}$$

Part II: For all $j = 0,1,2$ and $i = 1,2,3,4$ satisfying $2j + i \leq 4$ there exists a constant $C > 0$ such that for all $x \in \mathbb{R}$, $t > 0$, and $u_0 \in \mathcal{W}^4$,

$$\left| \frac{\partial^j}{\partial t^j} \frac{\partial^i}{\partial x^i} u(t,x) \right| \leq \frac{C}{\sqrt{t}} \left\| u_0' \right\|_{\gamma,1}, \tag{2.19}$$

where $\gamma = 1$ if $2j+i = 1$ or 2; $\gamma = 2$ if $2j+i = 3$ or 4, and $\|g\|_{\gamma,1} = \sum_{i=1}^{\gamma} \left\| \frac{\partial^i g}{\partial x^i} \right\|_1$.

The proof of the theorem will be presented in Section 4 to keep the presentation more transparent.

3. Numerical Methods for Stochastic Diffusion in the Presence of an Interface

In this section we will consider a numerical solution to system (2.1) using a Monte-Carlo method. The discontinuities in the coefficient of the equation, as well as the generality of the interface condition considered in this paper present challenges in two different aspects of the theory. On the one hand, the discontinuity in the diffusion coefficient naturally requires to consider SDEs that include a local time term (see Section 2.1 for details). As noted in [30], a transformation of the stochastic process can be defined so that this local time term is eliminated. On the other hand, the generality of the interface condition here renders inadequate the approach of [30] since they benefited from the self adjoint property of the problem under their consideration. Instead, in the problem treated in this paper, a careful quantification of the effect of the interface condition is needed.

In what follows we will use the approach developed in [30] to eliminate the local time term in the SDE associated to solutions of (2.1), and introduce an Euler-Maruyama method to approximate solutions of the resulting SDE. We will construct an explicit one-to-one transformation which transforms $Y^{(\alpha)}$ to a solution to a stochastic differential equation without a local time which can easily be discretized by a standard Euler-Maruyama scheme. Since the transformation is one-to-one and explicit, we can take the inverse transformation of this numerical solution to obtain a numerical approximation for $Y^{(\alpha)}$. As a consequence of Theorem 3, we can approximate $u(t,x)$ by $\mathbb{E}^x u_0(Y^{(\alpha)}(t))$ and compute the latter using a Monte-Carlo simulation. The main theorems establishing the rate of convergence of the approximation are stated in this section, with proofs given in Section 4.

3.1. A Transformation

We denote

$$\beta(x) = \lambda x \mathbf{1}_{(-\infty,0]}(x) + (1-\lambda) x \mathbf{1}_{(0,\infty)}(x). \tag{3.1}$$

Then $\beta(\cdot)$ is a one-to-one mapping with the inverse $\beta^{-1}(x) = \frac{x}{\lambda}\mathbf{1}_{(-\infty,0]}(x) + \frac{x}{1-\lambda}\mathbf{1}_{(0,\infty)}(x)$. It is easy to see that $\beta'_-(x) = \lambda \mathbf{1}_{(-\infty,0]}(x) + (1-\lambda)\mathbf{1}_{(0,\infty)}(x)$ and $\lambda\beta'_-(0^+) = (1-\lambda)\beta'_-(0^-)$. Thus, $\beta \in C^2(\mathbb{R}\setminus\{0\}) \cap C(\mathbb{R})$.

Denote $\theta(x) = \beta'_-(x)\sqrt{D(x)}$. It follows that

$$\theta(x) := \beta'_-(x)\sqrt{D(x)} = \lambda\sqrt{D^-}\mathbf{1}_{(-\infty,0]}(x) + (1-\lambda)\sqrt{D^+}\mathbf{1}_{(0,\infty)}(x). \tag{3.2}$$

Since $\beta \in C^2(\mathbb{R}\setminus\{0\}) \cap C(\mathbb{R})$ and $\theta \circ \beta = \beta'$, by using (2.15) and Itô-Tanaka formula we get

$$\begin{aligned} \beta\big(Y^{(\alpha)}(t)\big) &= \beta\big(Y^{(\alpha)}(0)\big) + \int_0^t \beta'_-\big(Y^{(\alpha)}(s)\big)\sqrt{D\big(Y^{(\alpha)}(s)\big)}dB(s) \\ &= \beta\big(Y^{(\alpha)}(0)\big) + \int_0^t \theta\Big(\beta\big(Y^{(\alpha)}(s)\big)\Big)dB(s). \end{aligned} \tag{3.3}$$

Denote $X(t) = \beta\big(Y^{(\alpha)}(t)\big)$, then (3.3) yields that $X(t)$ is a solution to a stochastic differential equation with piecewise constant diffusion coefficient

$$X(t) = X(0) + \int_0^t \theta(X(s))dB(s). \tag{3.4}$$

Note that the existence and uniqueness of (3.4) is proved in Theorem 1.3 (in which Assumption B holds) and the Remark thereafter in [43]. This equation will be useful to approximate the stochastic process $Y^{(\alpha)}(t)$ and therefore $u(t,x)$ by virtue of its stochastic representation (2.14).

3.2. Euler-Maruyama Scheme

Let M be a positive integer and $\Delta = \Delta t = \frac{T}{M}$ the step size. For $0 \le k \le M$, put $t_k = k\Delta t$. The Euler-Maruyama approximation $\bar{X}^{\Delta}(t)$ of $X(t)$ is defined as follows

$$\begin{aligned} &\bar{X}^{\Delta}(t) = \bar{X}^{\Delta}(t_k) + \theta\big(\bar{X}^{\Delta}(t_k)\big)\big(B(t) - B(t_k)\big), \quad t_k < t \le t_{k+1}, \\ &\bar{X}^{\Delta}(0) = \beta\big(Y^{(\alpha)}(0)\big). \end{aligned} \tag{3.5}$$

Algorithm A step of the Euler-Maruyama scheme

Data: The position $\bar{X}^{\Delta}(t_k)$ at time t_k of the process.
Result: The position $\bar{X}^{\Delta}(t_{k+1})$ at time t_{k+1} of the process.
if $\bar{X}^{\Delta}(t_k) \le 0$ **then**
  return $\bar{X}^{\Delta}(t_k) + \lambda\sqrt{D^-}\xi$ with $\xi \sim \mathrm{N}(0, \Delta t)$;
else
  return $\bar{X}^{\Delta}(t_k) + (1-\lambda)\sqrt{D^+}\xi$ with $\xi \sim \mathrm{N}(0, \Delta t)$;
end

Next, we can approximate $Y^{(\alpha)}(t)$ by inversely transforming $\bar{X}^{\Delta}(t)$

$$\bar{Y}^{\Delta}(t) = \beta^{-1}\big(\bar{X}^{\Delta}(t)\big), \qquad 0 \le t \le T. \tag{3.6}$$

The numerical solution to (2.1) can be now obtained. Define

$$u_{\Delta}(T, x) = \mathbb{E}^{x} u_0(\bar{Y}^{\Delta}(T)). \tag{3.7}$$

3.3. Convergence Rate

The convergence rate of the above numerical method is given in the following theorem.

Theorem 5. *For all initial condition $u_0 \in \mathcal{W}^4$, all parameter $0 < \epsilon < 1/2$ there exists a constant C depending on ϵ such that for all n large enough, and all $x_0 \in \mathbb{R}$,*

$$\Big|\mathbb{E}^{x_0} u_0(Y^{(\alpha)}(T)) - \mathbb{E}^{x_0} u_0(\bar{Y}^{\Delta}(T))\Big| \le C\|u_0'\|_{1,1}\Delta t^{(1-\epsilon)/2} + C\|u_0'\|_{1,1}\sqrt{\Delta t} + C\|u_0'\|_{3,1}\Delta t^{1-\epsilon}. \tag{3.8}$$

Next, we can relax the transmission conditions of u_0 and $\tilde{\mathcal{L}}u_0$ in the above theorem which are required in the definition of $\mathcal{W}_4$.

Theorem 6. *Let $u_0 : \mathbb{R} \to \mathbb{R}$ be in the space*

$$\mathcal{W} = \Big\{ g \in \mathcal{C}_b^4\big(\mathbb{R}\backslash\{0\}\big),\, g^{(i)} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}) \ \text{for}\ i = 1, \ldots, 4 \Big\}.$$

Then for any parameter $0 < \epsilon < 1/2$ there exists a constant C depending on u_0 and ϵ such that for all n large enough, and all $x_0 \in \mathbb{R}$,

$$\Big| u_{\Delta}(T, x_0) - u(T, x_0) \Big| \le C\Delta t^{1/2-\epsilon}. \tag{3.9}$$

The proof of these results will be given in the next section.

4. Proofs of Main Results

In this section we collectively present the proofs of Theorem 4, Theorem 5 and Theorem 6. To this end, the explicit formulae available for the transition probability density of skew Brownian motion and careful analysis of the error estimates are done. The convergence rate of Euler-Maruyama is proved using the approach by Martinez and Talay in [30]. As mentioned above, the interface conditions adopted in [30] makes the product of the diffusion coefficient and the first derivative of the solution a continuous function throughout the domain under consideration. In the present problem, we consider more general problems in which the product of the derivate of the solution and the diffusion coefficient remains discontinuous. This generality requires a more careful study of the error estimates in the Euler Muruyama method at the interface than the one required in [30].

4.1. Proof of Theorem **4**

The proof will follow from a sequence of steps involving lemmas.

Proof of Part I.

Let $p^{(\alpha)}(t,x,y)$ be the density function of the skew Brownian motion $B^{(\alpha)}$, then according to [19],

$$p^{(\alpha)}(t,x,y) = \begin{cases} \frac{1}{\sqrt{2\pi t}} e^{\frac{-(y-x)^2}{2t}} + \frac{(2\alpha-1)}{\sqrt{2\pi t}} e^{\frac{-(x+y)^2}{2t}}, & \text{if } x>0,\ y>0, \\ \frac{1}{\sqrt{2\pi t}} e^{\frac{-(y-x)^2}{2t}} - \frac{(2\alpha-1)}{\sqrt{2\pi t}} e^{\frac{-(x+y)^2}{2t}}, & \text{if } x<0,\ y<0, \\ \frac{2\alpha}{\sqrt{2\pi t}} e^{\frac{-(y-x)^2}{2t}}, & \text{if } x\le 0,\ y>0, \\ \frac{2(1-\alpha)}{\sqrt{2\pi t}} e^{\frac{-(y-x)^2}{2t}}, & \text{if } x\ge 0,\ y<0. \end{cases} \tag{4.1}$$

Thus, it follows from (2.9) that $Y^{(\alpha)}(t)$ under $\mathbb{P}^x$ has a density denoted by $q^{(\alpha)}(t,x,y)$ which satisfies

$$q^{(\alpha)}(t,x,y) = \frac{1}{\sqrt{D(y)}} p^{(\alpha)}\left(t, \frac{x}{\sqrt{D(x)}}, \frac{y}{\sqrt{D(y)}}\right). \tag{4.2}$$

It is clear that (4.1) and (4.2) imply (2.17) and then (2.18).

Proof of Part II. The proof is broken into a few lemma, estimating respectively time derivatives and space derivatives respectively. We begin by estimating the first partial derivative with respect to time.

Lemma 7. *There exists a positive constant C such that for all $t \in (0,T]$,*

$$\sup_{x\neq 0} \left| \frac{\partial u}{\partial t}(t,x) \right| \le \frac{C}{\sqrt{t}} \|u_0'\|_{1,1}. \tag{4.3}$$

Proof. Recall that (2.15) holds true for any $u_0 \in C_b^2(\mathbb{R}\setminus\{0\}) \cap C(\mathbb{R})$ satisfying $\lambda u_0'(0^+) = (1-\lambda)u_0'(0^-)$ and $u_0''(0^+) = u_0''(0^-)$. Hence, for all $x\in\mathbb{R}$ and $t>0$,

$$\mathbb{E}^x u_0\big(Y^{(\alpha)}(t)\big) = u_0(x) + \int_0^t \mathbb{E}^x \tilde{\mathcal{L}} u_0\big(Y^{(\alpha)}(s)\big) ds, \tag{4.4}$$

where the operator $\tilde{\mathcal{L}}$ is defined as in (2.10). In addition, notice that

$$dY^{(\alpha)}(t) = \sqrt{\big(Y^{(\alpha)}(t)\big)} dB(t) + \left(\frac{\sqrt{D^+} - \sqrt{D^-}}{2} + \sqrt{D^-}\frac{2\alpha-1}{2\alpha} \right) dl_t^{B^{(\alpha)},+}(0). \tag{4.5}$$

Fix $x > 0$. Denote $\tau_0(Y^{(\alpha)}) = \inf\{s > 0 : Y^{(\alpha)}(s) = 0\}$ and $r_0^x(s)$ the density of $\tau_0(Y^{(\alpha)}) \wedge T$ under $\mathbb{P}^x$. Notice that $\tau_0(Y^{(\alpha)}) = \tau_0\big(x + \sqrt{D^+}B\big)$ where $B(\cdot)$ is the standard Brownian motion. For any function h such that $\mathbb{E}^x h(Y^{(\alpha)}) < \infty$ we have

$$
\begin{aligned}
&\mathbb{E}^x h(Y^{(\alpha)}(t)) \\
&= \mathbb{E}^x\Big[h(Y^{(\alpha)}(t))\mathbf{1}_{\{\tau_0 \ge t\}}\Big] + \mathbb{E}^x\Big[h(Y^{(\alpha)}(t))\mathbf{1}_{\{\tau_0 < t\}}\Big] \\
&= \mathbb{E}^x\Big[h\big(x + \sqrt{D^+}B(t)\big)\mathbf{1}_{\{\tau_0 \ge t\}}\Big] + \int_0^t \mathbb{E}^0 h\big(Y^{(\alpha)}(t-s)\big) r_0^x(s)ds \\
&= \mathbb{E}^x h\big(x + \sqrt{D^+}B(t)\big) - \mathbb{E}^x\Big[h\big(x + \sqrt{D^+}B(t)\big)\mathbf{1}_{\{\tau_0 < t\}}\Big] + \int_0^t \mathbb{E}^0 h\big(Y^{(\alpha)}(t-s)\big) r_0^x(s)ds \\
&= \mathbb{E}^x h\big(x + \sqrt{D^+}B(t)\big) - \int_0^t \mathbb{E}^0 h\big(\sqrt{D^+}B(s)\big) r_0^x(t-s)ds + \int_0^t \mathbb{E}^0 h\big(Y^{(\alpha)}(s)\big) r_0^x(t-s)ds.
\end{aligned} \tag{4.6}
$$

For $x < 0$ we have a similar identity. To proceed, we assume that $x > 0$. From (4.6) we can write

$$
u(t,x) = \mathbb{E}^x u_0(Y^{(\alpha)}(t)) = \mathbb{E}^x u_0\big(x + \sqrt{D^+}B(t)\big) + v(t,x), \tag{4.7}
$$

where

$$
\begin{aligned}
v(t,x) &= -\int_0^t \mathbb{E}^0 u_0\big(\sqrt{D^+}B(s)\big) r_0^x(t-s)ds + \int_0^t \mathbb{E}^0 u_0\big(Y^{(\alpha)}(s)\big) r_0^x(t-s)ds \\
&= \int_0^t \int_0^s \Big[\mathbb{E}^0 \tilde{\mathcal{L}} u_0\big(Y^{(\alpha)}(\xi)\big) - \mathbb{E}^0 \tilde{\mathcal{L}}^+ u_0\big(\sqrt{D^+}B(\xi)\big)\Big] d\xi \; r_0^x(t-s)ds
\end{aligned} \tag{4.8}
$$

and $\tilde{\mathcal{L}}^+ u_0 = \frac{D^+}{2} u_0''$. Since

$$
\frac{\partial v}{\partial t}(t,x) = \int_0^t \Big[\mathbb{E}^0 \tilde{\mathcal{L}} u_0\big(Y^{(\alpha)}(s)\big) - \mathbb{E}^0 \tilde{\mathcal{L}}^+ u_0\big(\sqrt{D^+}B(s)\big)\Big] r_0^x(t-s)ds, \tag{4.9}
$$

according to Part I of Theorem 2.4 and Lemma 10 we obtain,

$$
\begin{aligned}
\left|\frac{\partial v}{\partial t}(t,x)\right| &\le \int_0^t \Big[\Big|\mathbb{E}^0 \tilde{\mathcal{L}} u_0\big(Y^{(\alpha)}(s)\big)\Big| + \Big|\mathbb{E}^0 \tilde{\mathcal{L}}^+ u_0\big(\sqrt{D^+}B(s)\big)\Big|\Big] r_0^x(t-s)ds \\
&\le C\Big(\big\|\tilde{\mathcal{L}} u_0\big\|_1 + \big\|\tilde{\mathcal{L}}^+ u_0\big\|_1\Big) \int_0^t \frac{1}{\sqrt{s}} r_0^x(t-s)ds \\
&\le \frac{C}{\sqrt{t}}\Big(\big\|\tilde{\mathcal{L}} u_0\big\|_1 + \big\|\tilde{\mathcal{L}}^+ u_0\big\|_1\Big).
\end{aligned} \tag{4.10}
$$

Next we estimate $\frac{\partial}{\partial t}\mathbb{E}^x u_0(x+\sqrt{D^+}B(t))$. It is obvious that the density $q^+(t,x,y)$ of $x + \sqrt{D^+}B(t)$ satisfies the inequality $q^+(t,x,y) \le \frac{C}{\sqrt{t}} \exp\{-\frac{(y-x)^2}{\nu t}\}$ for all $0 \le t \le T$ for some constants C, ν. It follows from the equation

$$
\frac{\partial}{\partial t}\mathbb{E}^x u_0\big(x+\sqrt{D^+}B(t)\big) = \mathbb{E}^x \tilde{\mathcal{L}}^+\Big(u_0\big(x+\sqrt{D^+}B(t)\big)\Big) = \frac{D^+}{2}\int u_0''(y) q^+(t,x,y)dy
$$

that

$$\sup_{x\in\mathbb{R}}\left|\frac{\partial}{\partial t}\mathbb{E}^x u_0(x+\sqrt{D^+}B(t))\right| \le \frac{C}{\sqrt{t}}\left\|\tilde{\mathcal{L}}^+ u_0\right\|_1. \tag{4.11}$$

Combining (4.7), (4.10), and (4.11) we derive (4.3) as desired. □

For the second time derivative we have the following.

Lemma 8. *There exists a positive constant C such that for all $t \in (0,T]$,*

$$\sup_{x\neq 0}\left|\frac{\partial^2 u}{\partial t^2}(t,x)\right| \le \frac{C}{\sqrt{t}}\|u_0'\|_{3,1}. \tag{4.12}$$

Proof. For $u_0 \in \mathcal{W}^4$, $\tilde{\mathcal{L}}u_0 \in \mathcal{W}^2$. By virtue of (4.7) and (4.9) we have

$$\begin{aligned}
\frac{\partial^2 u}{\partial t^2}(t,x) &= \frac{\partial^2}{\partial t^2}\mathbb{E}^x u_0\big(x+\sqrt{D^+}B(t)\big)\\
&\quad + \int_0^t \frac{\partial}{\partial t}\left[\mathbb{E}^0\tilde{\mathcal{L}}u_0\big(Y^{(\alpha)}(t-s)\big) - \mathbb{E}^0\tilde{\mathcal{L}}^+u_0\big(\sqrt{D^+}B(t-s)\big)\right] r_0^x(s)ds\\
&= \frac{\partial}{\partial t}\mathbb{E}^x\tilde{\mathcal{L}}^+u_0\big(x+\sqrt{D^+}B(t)\big)\\
&\quad + \int_0^t \left[\mathbb{E}^0\tilde{\mathcal{L}}(\tilde{\mathcal{L}}u_0)\big(Y^{(\alpha)}(s)\big) - \mathbb{E}^0\tilde{\mathcal{L}}^+(\tilde{\mathcal{L}}^+u_0)\big(\sqrt{D^+}B(s)\big)\right] r_0^x(t-s)ds.
\end{aligned}$$

Therefore, by Lemma 7, we obtain

$$\left|\frac{\partial^2 u}{\partial t^2}(t,x)\right| \le \frac{C}{\sqrt{t}}\left\|\tilde{\mathcal{L}}^+(\tilde{\mathcal{L}}^+u_0)\right\|_1 + \frac{C}{\sqrt{t}}\left(\|\tilde{\mathcal{L}}(\tilde{\mathcal{L}}u_0)\|_1 + \|\tilde{\mathcal{L}}^+(\tilde{\mathcal{L}}^+u_0)\|_1\right) = \frac{C}{\sqrt{t}}\|u_0'\|_{3,1}.$$

For spatial derivatives, we first establish the following estimate.

Lemma 9. *There exists a positive constant C such that for all $t \in (0,T]$,*

$$\sup_{x\neq 0}\left|\frac{\partial u}{\partial x}(t,x)\right| \le \frac{C}{\sqrt{t}}\|u_0'\|_{1,1}. \tag{4.13}$$

Proof. Since $\frac{\partial}{\partial x}\mathbb{E}^x u_0(x+\sqrt{D^+}B(t)) = \mathbb{E}^x u_0'(x+\sqrt{D^+}B(t))$, we have

$$\begin{aligned}
\left\|\frac{\partial}{\partial x}\mathbb{E}^x u_0(x+\sqrt{D^+}B(t))\right\|_\infty &= \left\|\mathbb{E}^x u_0'(x+\sqrt{D^+}B(t))\right\|_\infty\\
&= \left\|\int u_0'(y)q^+(t,x,y)dy\right\|_\infty\\
&\le \frac{C}{\sqrt{t}}\left\|\int u_0'(y)e^{-\frac{(y-x)^2}{D^+t^2}}dy\right\|_\infty \le \frac{C}{\sqrt{t}}\|u_0'\|_1.
\end{aligned} \tag{4.14}$$

Let

$$H(s) = \int_0^s \Big[\mathbb{E}^0 \tilde{\mathcal{L}} u_0(Y^{(\alpha)}(\xi)) - \mathbb{E}^0 \tilde{\mathcal{L}}^+ u_0(x + \sqrt{D^+} B(\xi))\Big]\, d\xi,$$

then since $H(0) = 0$ and $H'(s) \le C\big(\|\tilde{\mathcal{L}} u_0\|_1 + \|\tilde{\mathcal{L}}^+ u_0\|_1\big) = \frac{C_H}{s^0}$ we have by (4.8) and Lemma 11 that

$$v(t,x) = \int_0^t H(s) r_0^x(t-s) ds$$

and

$$\Big|\frac{\partial v}{\partial x}(t,x)\Big| \le \tilde{C}\big(\|\tilde{\mathcal{L}}^+ u_0\|_1 + \|\tilde{\mathcal{L}} u_0\|_1\big). \tag{4.15}$$

In view of (4.7), (4.14) and (4.15) we obtain (4.13). □

By the similar way we can prove the estimates for $\Big|\frac{\partial^j}{\partial t^j}\frac{\partial^i}{\partial x^i} u(t,x)\Big|$ for $2j+i \le 4$. □

4.2. Proof of Theorem **5**

Denote $s_k = T - t_k$ for $0 \le k \le M$. Since $u(0,x) = u_0(x)$ and $u(T,x) = \mathbb{E}^x u_0(Y^{(\alpha)}(T))$,

$$\begin{aligned}
&u(0, \beta^{-1}(\bar{X}^\Delta(T)) = u_0(\beta^{-1}(\bar{X}^\Delta(T))),\\
&u(T, x_0) = u(T, \bar{X}^\Delta(0)) = u(T, \beta^{-1}(Y^{(\alpha)}(0)) = \mathbb{E}^{x_0} u_0(Y^{(\alpha)}(T)).
\end{aligned}$$

Therefore,

$$\begin{aligned}
\epsilon_T^{x_0} &= \Big|\mathbb{E}^{x_0} u_0\big(Y^{(\alpha)}(T)\big) - \mathbb{E}^{x_0} u_0\big(\bar{Y}^\Delta(T)\big)\Big| = \Big|\mathbb{E}^{x_0} u_0\big(\beta^{-1}(\bar{X}(T))\big) - \mathbb{E}^{x_0} u_0\big(\beta^{-1}(\bar{X}^\Delta(T))\big)\Big|\\
&= \Big|\mathbb{E}^{x_0} u\big(T, \beta^{-1}(\bar{X}^\Delta(0))\big) - \mathbb{E}^{x_0} u\big(0, \beta^{-1}(\bar{X}^\Delta(T))\big)\Big|\\
&= \Big|\sum_{k=0}^{M-1}\Big[\mathbb{E}^{x_0} u\big(T - t_k, \beta^{-1}(\bar{X}^\Delta(t_k))\big) - \mathbb{E}^{x_0} u\big(T - t_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_{k+1}))\big)\Big]\Big|\\
&\le \Big|\sum_{k=0}^{M-2}\Big[\mathbb{E}^{x_0} u\big(s_k, \beta^{-1}(\bar{X}^\Delta(t_k))\big) - \mathbb{E}^{x_0} u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_{k+1}))\big)\Big]\Big|\\
&\quad + \Big|\mathbb{E}^{x_0} u\big(s_{M-1}, \beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big) - \mathbb{E}^{x_0} u\big(0, \beta^{-1}(\bar{X}^\Delta(T))\big)\Big|.
\end{aligned} \tag{4.16}$$

To estimate the second term in (4.16), we use the fact that $u(0,x) = u_0(x)$ and obtain

$$\begin{aligned}
&\Big|\mathbb{E}^{x_0} u\big(s_{M-1}, \beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big) - \mathbb{E}^{x_0} u\big(0, \beta^{-1}(\bar{X}^\Delta(T))\big)\Big|\\
&\quad \le \Big|\mathbb{E}^{x_0} u\big(s_{M-1}, \beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big) - \mathbb{E}^{x_0} u\big(0, \beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big)\Big|\\
&\qquad + \Big|\mathbb{E}^{x_0} u_0\big(\beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big) - \mathbb{E}^{x_0} u_0\big(\beta^{-1}(\bar{X}^\Delta(T))\big)\Big|.
\end{aligned}$$

Since u_0'' is in $L_1(\mathbb{R})$, u_0' is bounded and $u_0 \circ \beta^{-1}$ is Lipschitz. By virtue of the inequality $\sup_{x\neq 0} |\frac{\partial u}{\partial t}(t,x)| \leq \frac{C}{\sqrt{t}}\|u_0'\|_{1,1}$ we have

$$\Big|\mathbb{E}^{x_0} u\big(s_{M-1}, \beta^{-1}(\bar{X}^\Delta(t_{M-1}))\big) - \mathbb{E}^{x_0} u\big(0, \beta^{-1}(\bar{X}^\Delta(T))\big)\Big| \leq C\|u_0'\|_{1,1}\sqrt{\Delta t}. \tag{4.17}$$

It remains to estimate the first term in (4.16). To proceed, we denote the time and space increments as follows

$$\begin{aligned} T_k &= u\big(s_k, \beta^{-1}(\bar{X}^\Delta(t_k))\big) - u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big), \\ S_k &= u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_{k+1}))\big) - u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big). \end{aligned}$$

The first term in (4.16) then can be rewritten as $\big|\sum_{k=0}^{M-2} \mathbb{E}^{x_0}(T_k - S_k)\big|$. The analysis of this term will be divided into 4 steps.

Step 1: Estimate for the time increment T_k: Since $s_k - s_{k+1} = \Delta t$, by the definition of T_k and applying a Taylor expansion we have

$$\begin{aligned} &\Big[u\big(s_k, \beta^{-1}(\bar{X}^\Delta(t_k))\big) - u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\Big] 1_{\{\bar{X}^\Delta(t_k)>0\}} \\ &= \Delta t \frac{\partial u}{\partial t}\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big) 1_{\{\bar{X}^\Delta(t_k)>0\}} \\ &\quad + \Delta t^2 \int_{[0,1]^2} \frac{\partial^2 u}{\partial t^2}\big(s_{k+1} + \tau_1\tau_2\Delta t, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\tau_1 d\tau_1 d\tau_2 1_{\{\bar{X}^\Delta(t_k)>0\}} \\ &= T_k^+ + R_k^+. \end{aligned}$$

Similarly,

$$\begin{aligned} &\Big[u\big(s_k, \beta^{-1}(\bar{X}^\Delta(t_k))\big) - u\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\Big] 1_{\{\bar{X}^\Delta(t_k)<0\}} \\ &= \Delta t \frac{\partial u}{\partial t}\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big) 1_{\{\bar{X}^\Delta(t_k)<0\}} \\ &\quad + \Delta t^2 \int_{[0,1]^2} \frac{\partial^2 u}{\partial t^2}\big(s_{k+1} + \tau_1\tau_2\Delta t, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\tau_1 d\tau_1 d\tau_2 1_{\{\bar{X}^\Delta(t_k)<0\}} \\ &= T_k^- + R_k^-. \end{aligned}$$

It follows from the above equations and the inequality $\sup_{x\neq 0} |\frac{\partial^2 u}{\partial t^2}(t,x)| \leq \frac{C}{\sqrt{t}}\|u_0'\|_{3,1}$ that

$$\mathbb{E}^{x_0}\big|R_k^+ + R_k^-\big| = \mathbb{E}^{x_0}\Delta t^2 \Big|\int_{[0,1]^2} \frac{\partial^2 u}{\partial t^2}\big(s_{k+1} + \tau_1\tau_2\Delta t, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\tau_1 d\tau_1 d\tau_2\Big| \leq \frac{C\Delta t^2}{\sqrt{s_{k+1}}}\|u_0'\|_{3,1}.$$

Therefore, we obtain

$$\mathbb{E}^{x_0} T_k = \Delta t \mathbb{E}^{x_0}\Big[\frac{\partial u}{\partial t}\big(s_{k+1}, \beta^{-1}(\bar{X}^\Delta(t_k))\big)\Big] + O\left(\frac{\Delta t^2}{\sqrt{s_{k+1}}}\right). \tag{4.18}$$

Step 2: Estimate for the space increment S_k: Let us denote the following increments, with θ as defined in (3.2)

$$\begin{aligned}\triangle_{k+1}B &= B(t_{k+1}) - B(t_k),\\ \triangle_{k+1}\bar{X}^{\Delta} &= \theta\big(\bar{X}^{\Delta}(t_k)\big)\triangle_{k+1}B,\\ \tilde{\triangle}_{k+1}\bar{Y}^{\Delta} &= \frac{\triangle_{k+1}\bar{X}^{\Delta}}{1-\lambda}1_{\{\bar{X}^{\Delta}(t_k)>0\}} + \frac{\triangle_{k+1}\bar{X}^{\Delta}}{\lambda}1_{\{\bar{X}^{\Delta}(t_k)<0\}},\end{aligned} \tag{4.19}$$

and events

$$\Omega_k^{++} = \Big\{\bar{X}^{\Delta}(t_k) > 0, \bar{X}^{\Delta}(t_{k+1}) > 0\Big\}, \quad \Omega_k^{+-} = \Big\{\bar{X}^{\Delta}(t_k) > 0, \bar{X}^{\Delta}(t_{k+1}) \le 0\Big\},$$
$$\Omega_k^{--} = \Big\{\bar{X}^{\Delta}(t_k) \le 0, \bar{X}^{\Delta}(t_{k+1}) \le 0\Big\}, \quad \Omega_k^{-+} = \Big\{\bar{X}^{\Delta}(t_k) \le 0, \bar{X}^{\Delta}(t_{k+1}) > 0\Big\}.$$

Hence, by the definition of the function β, on Ω_k^{++},

$$\beta^{-1}\big(\bar{X}^{\Delta}(t_{k+1})\big) = \beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big) + \frac{\triangle_{k+1}\bar{X}^{\Delta}}{1-\lambda}.$$

This and a Taylor expansion yield

$$\begin{aligned}&S_k 1_{\Omega_k^{++}}\\ &= \frac{\triangle_{k+1}\bar{X}^{\Delta}}{1-\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{++}} + \frac{1}{2}\frac{(\triangle_{k+1}\bar{X}^{\Delta})^2}{(1-\lambda)^2}\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{++}}\\ &\quad + \frac{1}{6}\frac{(\triangle_{k+1}\bar{X}^{\Delta})^3}{(1-\lambda)^3}\frac{\partial^3 u}{\partial x^3}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{++}}\\ &\quad + \frac{(\triangle_{k+1}\bar{X}^{\Delta})^4}{(1-\lambda)^4}\int_{[0,1]^4}\frac{\partial^4 u}{\partial x^4}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k)) + \tau_1\tau_2\tau_3\tau_4\frac{\triangle_{k+1}\bar{X}^{\Delta}}{1-\lambda}\Big)\tau_1\tau_2\tau_3 d\tau_1\dots d\tau_4 1_{\Omega_k^{++}}\\ &=: S_k^{++1} + S_k^{++2} + S_k^{++3} + S_k^{++4}.\end{aligned}$$

Similarly,

$$\begin{aligned}&S_k 1_{\Omega_k^{--}}\\ &= \frac{\triangle_{k+1}\bar{X}^{\Delta}}{\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{--}} + \frac{1}{2}\frac{(\triangle_{k+1}\bar{X}^{\Delta})^2}{\lambda^2}\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{--}}\\ &\quad + \frac{1}{6}\frac{(\triangle_{k+1}\bar{X}^{\Delta})^3}{\lambda^3}\frac{\partial^3 u}{\partial x^3}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\Omega_k^{--}}\\ &\quad + \frac{(\triangle_{k+1}\bar{X}^{\Delta})^4}{\lambda^4}\int_{[0,1]^4}\frac{\partial^4 u}{\partial x^4}\Big(s_{k+1}, \beta^{-1}(\bar{X}^{\Delta}(t_k)) + \tau_1\tau_2\tau_3\tau_4\frac{\triangle_{k+1}\bar{X}^{\Delta}}{\lambda}\Big)\tau_1\tau_2\tau_3 d\tau_1\dots d\tau_4 1_{\Omega_k^{--}}\\ &=: S_k^{--1} + S_k^{--2} + S_k^{--3} + S_k^{--4}.\end{aligned}$$

Since $\Omega_k^{++}\cup\Omega_k^{--} = \Omega - \big(\Omega_k^{+-}\cup\Omega_k^{-+}\big)$ and $\Omega_k^{+-}\cup\Omega_k^{-+} \in \sigma\{B(t) : 0 \le t \le t_{k+1}\}$, by (4.19) we get

$$
\begin{aligned}
&\mathbb{E}^{x_0}\Big(S_k^{++1}+S_k^{--1}\Big)\\
&=\mathbb{E}^{x_0}\left[\frac{\triangle_{k+1}\bar{X}^\Delta}{1-\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\Omega_k^{++}}+\frac{\triangle_{k+1}\bar{X}^\Delta}{\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\Omega_k^{--}}\right]\\
&\quad+\mathbb{E}^{x_0}\left[\tilde{\triangle}_{k+1}\bar{Y}^\Delta\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]\\
&\quad-\mathbb{E}^{x_0}\left[\tilde{\triangle}_{k+1}\bar{Y}^\Delta\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]\\
&=\mathbb{E}^{x_0}\left[\Big(\frac{\triangle_{k+1}\bar{X}^\Delta}{1-\lambda}1_{\{\bar{X}^\Delta(t_k)>0\}}+\frac{\triangle_{k+1}\bar{X}^\Delta}{\lambda}1_{\{\bar{X}^\Delta(t_k)<0\}}\Big)\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)\right]\\
&\quad-\mathbb{E}^{x_0}\left[\tilde{\triangle}_{k+1}\bar{Y}^\Delta\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]\\
&=-\mathbb{E}^{x_0}\left[\tilde{\triangle}_{k+1}\bar{Y}^\Delta\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right].
\end{aligned}\tag{4.20}
$$

In the last step we have used that

$$
\frac{\triangle_{k+1}\bar{X}^\Delta}{1-\lambda}1_{\{\bar{X}^\Delta(t_k)>0\}}+\frac{\triangle_{k+1}\bar{X}^\Delta}{\lambda}1_{\{\bar{X}^\Delta(t_k)<0\}}=\Big[\sqrt{D^+}1_{\{\bar{X}^\Delta(t_k)>0\}}+\sqrt{D^-}1_{\{\bar{X}^\Delta(t_k)<0\}}\Big]\Delta_{k+1}B
$$

so by conditioning, we get that its expectation vanishes.

In a similar manner, and using that $\mathbb{E}\big[(\triangle_{k+1}B)^2\big|\,B(t),\,0\le t\le t_k\big]=\Delta t$, we obtain

$$
\begin{aligned}
&\mathbb{E}^{x_0}\Big(S_k^{++2}+S_k^{--2}\Big)\\
&=\frac{1}{2}\mathbb{E}^{x_0}\left\{\left[\Big(\frac{\triangle_{k+1}\bar{X}^\Delta}{1-\lambda}\Big)^2 1_{\Omega_k^{++}}+\Big(\frac{\triangle_{k+1}\bar{X}^\Delta}{\lambda}\Big)^2 1_{\Omega_k^{--}}\right]\frac{\partial^2 u}{\partial x^2}\big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\big)\right\}\\
&=\frac{1}{2}\mathbb{E}^{x_0}\Bigg\{\left[\Big(\frac{\theta(\bar{X}^\Delta(t_k))\triangle_{k+1}B}{1-\lambda}\Big)^2 1_{\{\bar{X}^\Delta(t_k)>0\}}+\Big(\frac{\theta(\bar{X}^\Delta(t_k))\triangle_{k+1}B}{\lambda}\Big)^2 1_{\{\bar{X}^\Delta(t_k)<0\}}\right]\\
&\quad\times\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)\Bigg\}-\frac{1}{2}\mathbb{E}^{x_0}\left[\big(\tilde{\triangle}_{k+1}\bar{Y}^\Delta\big)^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]\\
&=\frac{\Delta t}{2}\mathbb{E}^{x_0}\left\{\big[D^+1_{\{\bar{X}^\Delta(t_k)>0\}}+D^-1_{\{\bar{X}^\Delta(t_k)<0\}}\big]\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)\right\}\\
&\quad-\frac{1}{2}\mathbb{E}^{x_0}\left[\big(\tilde{\triangle}_{k+1}\bar{Y}^\Delta\big)^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]\\
&=\frac{\Delta t}{2}\mathbb{E}^{x_0}\left[D\big(\beta^{-1}(\bar{X}^\Delta(t_k))\big)\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)\right]\\
&\quad-\frac{1}{2}\mathbb{E}^{x_0}\left[\big(\tilde{\triangle}_{k+1}\bar{Y}^\Delta\big)^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right].
\end{aligned}
$$

Thus,

$$\mathbb{E}^{x_0}\Big(S_k^{++2}+S_k^{--2}\Big)=\mathbb{E}^{x_0}\tilde{\mathcal{L}}u\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)\Delta t \\ -\frac{1}{2}\mathbb{E}^{x_0}\left[(\tilde{\triangle}_{k+1}\bar{Y}^{\Delta})^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]. \tag{4.21}$$

Since $\mathbb{E}\big[(\triangle_{k+1}B)^3\big|\,B(t),\,0\le t\le t_k\big]=0$,

$$\mathbb{E}^{x_0}\Big(S_k^{++3}+S_k^{--3}\Big)=-\frac{1}{6}\mathbb{E}^{x_0}\left[(\tilde{\triangle}_{k+1}\bar{Y}^{\Delta})^3\frac{\partial^3 u}{\partial x^3}\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\right]. \tag{4.22}$$

Next, according to Theorem 4,

$$\mathbb{E}^{x_0}\Big|S_k^{++4}+S_k^{--4}\Big|\le\frac{C\Delta t^2}{\sqrt{s_{k+1}}}\big\|u_0'\big\|_{3,1}. \tag{4.23}$$

Combining the estimates (4.20) through (4.23) above, we arrive at

$$\begin{aligned}\mathbb{E}^{x_0}S_k&=\mathbb{E}^{x_0}\tilde{\mathcal{L}}u\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)\Delta t\\ &\quad+\mathbb{E}^{x_0}\Bigg\{\left[S_k-\tilde{\triangle}_{k+1}\bar{Y}^{\Delta}\frac{\partial u}{\partial x}\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)\right]1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\\ &\quad-\frac{1}{2}(\tilde{\triangle}_{k+1}\bar{Y}^{\Delta})^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\\ &\quad-\frac{1}{6}(\tilde{\triangle}_{k+1}\bar{Y}^{\Delta})^3\frac{\partial^3 u}{\partial x^3}\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)1_{\{\Omega_k^{+-}\cup\Omega_k^{-+}\}}\Bigg\}+O\left(\frac{\Delta t^2}{\sqrt{s_{k+1}}}\right)\\ &=:\mathbb{E}^{x_0}\tilde{\mathcal{L}}u\Big(s_{k+1},\beta^{-1}(\bar{X}^{\Delta}(t_k))\Big)\Delta t+\mathbb{E}^{x_0}\mathcal{R}_k+O\left(\frac{\Delta t^2}{\sqrt{s_{k+1}}}\right).\end{aligned} \tag{4.24}$$

We now estimate the remaining term $\mathbb{E}^{x_0}\mathcal{R}_k$.

Step 3: Estimate $\mathbb{E}^{x_0}\mathcal{R}_k$:

For any fixed $\epsilon\in(0,1/2)$, we will show that

$$\Big|\mathbb{E}^{x_0}\mathcal{R}_k\Big|\le\frac{C\Delta t^{1-2\epsilon}}{\sqrt{s_{k+1}}}\big\|u_0'\big\|_{1,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^{\Delta}(t_k)\big|\le\Delta t^{\frac{1}{2}-\epsilon}\Big\} \\ +\frac{C\Delta t^{\frac{3}{2}-3\epsilon}}{\sqrt{s_{k+1}}}\big\|u_0'\big\|_{3,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^{\Delta}(t_k)\big|\le\Delta t^{\frac{1}{2}-\epsilon}\Big\}. \tag{4.25}$$

Notice that we can rewrite Ω_k^{+-} as

$$\Omega_k^{+-}=\Big\{\bar{X}^{\Delta}(t_k)\ge\Delta t^{\frac{1}{2}-\epsilon},\ \bar{X}^{\Delta}(t_{k+1})\le 0\Big\}\cup\Big\{0<\bar{X}^{\Delta}(t_k)\le\Delta t^{\frac{1}{2}-\epsilon},\ \bar{X}^{\Delta}(t_{k+1})\le-\Delta t^{\frac{1}{2}-\epsilon}\Big\} \\ \cup\Big\{0<\bar{X}^{\Delta}(t_k)\le\Delta t^{\frac{1}{2}-\epsilon},\ -\Delta t^{\frac{1}{2}-\epsilon}\le\bar{X}^{\Delta}(t_{k+1})\le 0\Big\}.$$

Since $\bar{X}^\Delta(t_{k+1}) = \bar{X}^\Delta(t_k) + \theta\big(\bar{X}^\Delta(t_k)\big)B(\Delta t)$, it follows that

$$\mathbb{P}\Big\{\bar{X}^\Delta(t_k) \geq \Delta t^{\frac{1}{2}-\epsilon},\ \bar{X}^\Delta(t_{k+1}) \leq 0\Big\} \leq \mathbb{P}\Big\{(1-\lambda)\sqrt{D^+}B(\Delta t) \geq \Delta t^{\frac{1}{2}-\epsilon}\Big\} \leq C\exp\{-CM^\epsilon\}.$$

Similarly,

$$\mathbb{P}\Big\{0 < \bar{X}^\Delta(t_k) \leq \Delta t^{\frac{1}{2}-\epsilon},\ \bar{X}^\Delta(t_{k+1}) \leq -\Delta t^{\frac{1}{2}-\epsilon}\Big\} \leq C\exp\{-CM^\epsilon\}.$$

We can proceed analogously on the event Ω_k^{-+}. This leads us to limit to consider the events

$$\begin{aligned}\hat{\Omega}_k^{+-} &= \Big\{0 < \bar{X}^\Delta(t_k) \leq \Delta t^{\frac{1}{2}-\epsilon},\ -\Delta t^{\frac{1}{2}-\epsilon} \leq \bar{X}^\Delta(t_{k+1}) \leq 0\Big\},\\ \hat{\Omega}_k^{-+} &= \Big\{-\Delta t^{\frac{1}{2}-\epsilon} \leq \bar{X}^\Delta(t_k) < 0,\ 0 \leq \bar{X}^\Delta(t_{k+1}) \leq \Delta t^{\frac{1}{2}-\epsilon}\Big\}.\end{aligned}$$

Note that, by (4.19), $\tilde{\triangle}_{k+1}\bar{Y}^\Delta \leq C\Delta t^{1/2-\epsilon}$ on these sets. Hence, we have

$$\begin{aligned}&\left|\mathbb{E}^{x_0}\left[\big(\tilde{\triangle}_{k+1}\bar{Y}^\Delta\big)^2\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\hat{\Omega}_k^{+-}\cup\hat{\Omega}_k^{-+}\}}\right]\right|\\ &\quad\leq \frac{C\Delta t^{1-2\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{1,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^\Delta(t_k)\big| \leq \Delta t^{\frac{1}{2}-\epsilon}\Big\},\\ &\left|\mathbb{E}^{x_0}\left[\big(\tilde{\triangle}_{k+1}\bar{Y}^\Delta\big)^3\frac{\partial^3 u}{\partial x^3}\Big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\Big)1_{\{\hat{\Omega}_k^{+-}\cup\hat{\Omega}_k^{-+}\}}\right]\right|\\ &\quad\leq \frac{C\Delta t^{\frac{3}{2}-3\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{3,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^\Delta(t_k)\big| \leq \Delta t^{\frac{1}{2}-\epsilon}\Big\}.\end{aligned}$$

Therefore, it suffices to show that

$$\begin{aligned}&\left|\mathbb{E}^{x_0}\left[S_k - \tilde{\triangle}_{k+1}\bar{Y}^\Delta\frac{\partial u}{\partial x}\big(s_{k+1},\beta^{-1}(\bar{X}^\Delta(t_k))\big)\right]1_{\{\hat{\Omega}_k^{+-}\cup\hat{\Omega}_k^{-+}\}}\right|\\ &\quad\leq \frac{C\Delta t^{1-2\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{1,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^\Delta(t_k)\big| \leq \Delta t^{\frac{1}{2}-\epsilon}\Big\}.\end{aligned}\tag{4.26}$$

Step 4: Proof of (4.26)

Note that on the set $\hat{\Omega}_k^{+-}$, $\bar{X}^\Delta(t_k)$ and $\bar{X}^\Delta(t_{k+1})$ are both closed to 0. In addition, $\bar{X}^\Delta(t_k) > 0$ and $\bar{X}^\Delta(t_{k+1}) < 0$. Thus, we have

$$\beta^{-1}\big(\bar{X}^\Delta(t_k)\big) = \frac{\bar{X}^\Delta(t_k)}{1-\lambda},\quad \beta^{-1}\big(\bar{X}^\Delta(t_{k+1})\big) = \frac{\bar{X}^\Delta(t_{k+1})}{\lambda}.$$

Since $u(t,x)$ is continuous at 0, we get

$$\begin{aligned}
&\mathbb{E}^{x_0}\left[S_k - \tilde{\triangle}_{k+1}\bar{Y}^{\Delta}\frac{\partial u}{\partial x}\Big(s_{k+1}, \beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big)\Big)\right]1_{\hat{\Omega}_k^{+-}} \\
&= \frac{1}{\lambda}\mathbb{E}^{x_0}\left[\bar{X}^{\Delta}(t_{k+1})\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^-\Big)1_{\hat{\Omega}_k^{+-}}\right] - \frac{1}{1-\lambda}\mathbb{E}^{x_0}\left[\bar{X}^{\Delta}(t_k)\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^+\Big)1_{\hat{\Omega}_k^{+-}}\right] \\
&\quad - \mathbb{E}^{x_0}\left[\tilde{\triangle}_{k+1}\bar{Y}^{\Delta}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^+\Big)1_{\hat{\Omega}_k^{+-}}\right] \\
&\quad + \mathbb{E}^{x_0}\Bigg\{\Bigg[\Big(\beta^{-1}\big(\bar{X}^{\Delta}(t_{k+1})\big)\Big)^2\int_{[0,1]^2}\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1}, \tau_1\tau_2\beta^{-1}\big(\bar{X}^{\Delta}(t_{k+1})\big)\Big)\tau_1 d\tau_1 d\tau_2 \\
&\quad - \Big(\beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big)\Big)^2\int_{[0,1]^2}\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1}, \tau_1\tau_2\beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big)\Big)\tau_1 d\tau_1 d\tau_2 \\
&\quad - \tilde{\triangle}_{k+1}\bar{Y}^{\Delta}\beta^{-1}(\bar{X}^{\Delta}(t_k))\int_0^1\frac{\partial^2 u}{\partial x^2}\Big(s_{k+1}, \tau_1\beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big)\Big)d\tau_1\Bigg]1_{\hat{\Omega}_k^{+-}}\Bigg\}.
\end{aligned}$$

On one hand, since $|\beta^{-1}\big(\bar{X}^{\Delta}(t_k)\big)|$ and $|\beta^{-1}\big(\bar{X}^{\Delta}(t_{k+1})\big)| \le C\Delta t^{1/2-\epsilon}$ on $\hat{\Omega}_k^{+-}$, the absolute value of the last expectation in the right-hand side can be bounded from above by

$$\frac{C\Delta t^{1-2\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{1,1}\mathbb{P}^{x_0}\Big\{\big|\bar{X}^{\Delta}(t_k)\big| \le \Delta t^{\frac{1}{2}-\epsilon}\Big\}.$$

On the other hand, by (4.19), we can rewrite the sum of the first three terms in the right hand side as

$$\begin{aligned}
&\mathbb{E}^{x_0}\Bigg\{\Bigg[\frac{\bar{X}^{\Delta}(t_{k+1})}{\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^-\Big) - \frac{\bar{X}^{\Delta}(t_k)}{1-\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^+\Big) \\
&\qquad - \frac{\bar{X}^{\Delta}(t_{k+1}) - \bar{X}^{\Delta}(t_k)}{1-\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^+\Big)\Bigg]1_{\hat{\Omega}_k^{+-}}\Bigg\} \\
=&\mathbb{E}^{x_0}\left\{\left[\frac{1}{\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^-\Big) - \frac{1}{1-\lambda}\frac{\partial u}{\partial x}\Big(s_{k+1}, 0^+\Big)\right]\bar{X}^{\Delta}(t_{k+1})1_{\hat{\Omega}_k^{+-}}\right\} = 0
\end{aligned}$$

by the interface condition. By the same way, we can proceed for the set $\hat{\Omega}_k^{-+}$. Then (4.26) follows and we obtain (4.25) as a consequence.

Combining (4.16)-(4.18), (4.24), (4.25) we arrive at

$$\begin{aligned}
\epsilon_T^{x_0} \le C\sum_{k=0}^{M-2}&\left[\frac{\Delta t^{1-2\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{1,1} + \frac{\Delta t^{\frac{3}{2}-3\epsilon}}{\sqrt{s_{k+1}}}\|u_0'\|_{3,1}\right]\mathbb{P}^{x_0}\Big\{\big|\bar{X}^{\Delta}(t_k)\big| \le \Delta t^{\frac{1}{2}-\epsilon}\Big\} \\
&+ C\|u_0'\|_{1,1}\Delta t^{\frac{1}{2}} + C\|u_0'\|_{3,1}\Delta t.
\end{aligned}$$

Next, to handle the right hand side of the above inequality we use [44, Theorem 1.2] which estimates the visits to a small ball by the process $\bar{X}^{\Delta}$. Using the notations in [44] we take $\xi = 0$, $b(t) \equiv 0$, $\sigma(t) = \theta\big(\bar{X}^\Delta(t_k)\big)$ for $t_k \le t \le t_{k+1}$, $f(t) = 1/\sqrt{T-t}$, and $h = \Delta t$. Since $\theta(\cdot)$ is bounded, we can easily check that Assumption 1.1 and Assumption 1.2 in [44] are both satisfied. It then follows by [44, Theorem 1.2] that there is a constant M_0 such that for $M \ge M_0$, the right hand side in the above inequality is bounded above by $C\|u_0'\|_{1,1}\Delta t^{(1-\epsilon)/2} + C\|u_0'\|_{1,1}\Delta t^{1/2} + C\|u_0'\|_{3,1}\Delta t$. This proves the theorem. $\square$

4.3. Proof of Theorem **6**

Let u_0 be any function in $\mathcal{W}$, and $0 < \delta < 1$ we will first approximate u_0 by a function u_δ in $\mathcal{W}^4$ such that

$$\begin{cases} u_\delta(x) = u_0(x) & \text{for } |x| > 2\delta, \\ u_\delta(x) = u_0(0) & \text{for } -\delta \le x \le \delta \end{cases} \quad \text{and} \quad \begin{cases} u_\delta^{(i)}(2\delta) = u_0^{(i)}(2\delta), \\ u_\delta^{(i)}(-2\delta) = u_0^{(i)}(-2\delta), \\ u_\delta^{(i)}(-\delta) = u_\delta^{(i)}(\delta) = 0 \end{cases} \quad \text{for } 1 \le i \le 4.$$

For $\delta \le x \le 2\delta$ denote

$$\begin{aligned} u_\delta(x) =& u_0(0) + \big(u_0(2\delta) - u_0(0)\big)p_0\big(\frac{x-\delta}{\delta}\big) + \delta u_0^{(1)}(2\delta)p_1\big(\frac{x-\delta}{\delta}\big) \\ & + \delta^2 u_0^{(2)}(2\delta)p_2\big(\frac{x-\delta}{\delta}\big) + \delta^3 u_0^{(3)}(2\delta)p_3\big(\frac{x-\delta}{\delta}\big) + \delta^4 u_0^{(4)}(2\delta)p_4\big(\frac{x-\delta}{\delta}\big), \end{aligned}$$

and for $-2\delta \le x \le -\delta$ denote

$$\begin{aligned} u_\delta(x) =& u_0(0) + \big(u_0(-2\delta) - u_0(0)\big)p_0\big(-\frac{x+\delta}{\delta}\big) - \delta u_0^{(1)}(-2\delta)p_1\big(-\frac{x+\delta}{\delta}\big) \\ & + \delta^2 u_0^{(2)}(-2\delta)p_2\big(-\frac{x+\delta}{\delta}\big) - \delta^3 u_0^{(3)}(-2\delta)p_3\big(-\frac{x+\delta}{\delta}\big) + \delta^4 u_0^{(4)}(-2\delta)p_4\big(-\frac{x+\delta}{\delta}\big), \end{aligned}$$

where $p_j(x)$, $0 \le j \le 4$, are polynomials on $[0,1]$ satisfying the following interpolation problem

$$p_j^{(i)}(0) = 0, \quad p_j^{(i)}(1) = \delta_{ij} \text{ for } 0 \le i, j \le 4,$$

where δ_{ij} is the Kronecker symbol. We can choose

$$\begin{aligned} p_0(x) &= x^5(70x^4 - 315x^3 + 540x^2 - 420x + 126), \\ p_1(x) &= x^5(1-x)(35x^3 - 120x^2 + 140x - 56), \\ p_2(x) &= \frac{1}{2}x^5(1-x)^2(15x^2 - 35x + 21), \\ p_3(x) &= \frac{1}{6}x^5(1-x)^3(5x - 6), \\ p_4(x) &= \frac{1}{24}x^5(1-x)^4, \end{aligned}$$

which satisfy

$$\Big\|p_j^{(i)}\Big(\frac{\cdot - \delta}{\delta}\Big)\Big\|_{L^1([\delta,2\delta])} + \Big\|p_j^{(i)}\Big(-\frac{\cdot + \delta}{\delta}\Big)\Big\|_{L^1([-2\delta,-\delta])} \le C\delta^{1-i}, \quad \forall\, i = 1, \ldots, 4$$

and imply

$$\|u_0 - u_\delta\|_1 = \int_{-2\delta}^{2\delta} |u_0(y) - u_0(0) + u_0(0) - u_\delta(y)| dy \le C\delta^2.$$

Similarly, there is a constant only depends on u_0 such that

$$\|u_0^{(i)} - u_\delta^{(i)}\|_1 \le C\delta^{2-i} \quad \forall\, i = 1, \ldots, 4. \tag{4.27}$$

Next, we will use the approximation u_δ of u_0 to estimate the error ϵ_T^x. We have

$$\begin{aligned}
\epsilon_T^x &= \left|\mathbb{E}^x u_0\big(Y^{(\alpha)}(T)\big) - \mathbb{E}^x u_0\big(\bar{Y}^\Delta(T)\big)\right| \\
&\le \left|\mathbb{E}^x u_0\big(Y^{(\alpha)}(T)\big) - \mathbb{E}^x u_\delta\big(Y^{(\alpha)}(T)\big)\right| + \left|\mathbb{E}^x u_\delta\big(Y^{(\alpha)}(T)\big) - \mathbb{E}^x u_\delta\big(\bar{Y}^\Delta(T)\big)\right| \\
&\quad + \left|\mathbb{E}^x u_\delta\big(\bar{Y}^\Delta(T)\big) - \mathbb{E}^x u_0\big(\bar{Y}^\Delta(T)\big)\right| \\
&\le I_1(\delta) + I_2(\delta) + I_3(\delta).
\end{aligned} \tag{4.28}$$

It follows from (2.17) that

$$I_1(\delta) \le \int_{-\infty}^{\infty} |u_0(y) - u_\delta(y)| q^{(\alpha)}(T,x,y) dy \le C\delta \int_{-2\delta}^{2\delta} q^{(\alpha)}(T,x,y) dy \le C\delta^2. \tag{4.29}$$

By virtue of Theorem 5 and (4.27), there are constants C depending only on u such that

$$I_2(\delta) \le C\|u_\delta'\|_{1,1}\Delta t^{1/2-\epsilon} + C\|u_\delta'\|_{1,1}\Delta t^{1/2} + \|u_\delta'\|_{3,1}\Delta t^{1-\epsilon} \le C\Delta t^{1/2-\epsilon} + C\delta^{-2}\Delta t^{1-\epsilon}. \tag{4.30}$$

To proceed, we need to estimate $I_3(\delta)$. Let χ be a function in $C^\infty(\mathbb{R})$ such that

$$\chi(x) \ge 1 \quad \forall\, |x| \le 1, \quad \text{and} \quad \chi^{(i)}(0) = 0, \quad \forall\, i = 1, \ldots, 4.$$

Denote $\chi_\delta(x) = \chi(\frac{x}{2\delta})$ then $\chi_\delta \ge \mathbf{1}_{[-2\delta,2\delta]}$, $\operatorname{supp}(\chi_\delta) = [-4\delta, 4\delta]$, and it is clear that $\chi, \chi_\delta \in \mathcal{W}^2$. In addition

$$\|\chi_\delta'\|_{1,1} \le \frac{C}{\delta} \quad \text{and} \quad \|\chi_\delta'\|_{3,1} \le \frac{C}{\delta^3}.$$

Thus, Theorem 5 and (2.17) yield

$$\begin{aligned}
\mathbb{P}^x\big(|\bar{Y}^\Delta(T)| \le 2\delta\big) &\le \mathbb{E}^x \chi_\delta(\bar{Y}^\Delta(T)) \\
&\le \left|\mathbb{E}^x \chi_\delta(\bar{Y}^\Delta(T)) - \mathbb{E}^x \chi_\delta(Y^{(\alpha)}(T))\right| + \mathbb{E}^x \chi_\delta(Y^{(\alpha)}(T)) \\
&\le C\Delta t^{\frac{1-\epsilon}{2}}\|\chi'\|_{1,1} + C\Delta t^{1-\epsilon}\|\chi'\|_{3,1} + \int_{-4\delta}^{4\delta} \chi_\delta(y) q^{(\alpha)}(t,x,y) dy \\
&\le C\frac{\Delta t^{\frac{1-\epsilon}{2}}}{\delta} + C\frac{\Delta t^{1-\epsilon}}{\delta^3} + \frac{C}{\sqrt{T}}\|\chi\|_\infty \delta
\end{aligned}$$

and

$$I_3(\delta) \leq C\delta\mathbb{P}^x\big(|\bar{Y}^\Delta(T)| \leq 2\delta\big) \leq C\Delta t^{\frac{1-\epsilon}{2}} + C\frac{\Delta t^{1-\epsilon}}{\delta^2} + \frac{C}{\sqrt{T}}\|\chi\|_\infty\delta^2. \quad (4.31)$$

By choosing the optimal value of the type Δt^γ of δ (with $\gamma = 1/4$), and combining (4.28)-(4.31), we obtain (3.8). $\square$

5. Numerical Examples

Consider the initial profile on the interval $[-5, 5]$ given by

$$u_0(x) = \begin{cases} (1-x^2)^5 & \text{if } |x| < 1, \\ 0 & \text{else.} \end{cases} \quad (5.1)$$

In this section, simulations are provided of the solution to (2.1) with (5.1) for two values of $D^+ \in \{10, 100\}$ while holding $D^- = 1$. We consider scenarios with $\lambda = \{\lambda^*, \lambda^\#\}$. The expected value solution formula from [14], and the SDE-Euler-Maruyama method discussed in Section 3, all computed at $t = 0.2$, are shown in Figure 1. For a comparison with deterministic numerical methods, we also plot the solution obtained with an immersed interface finite element method (IFEM) (see [45]) for the diffusion problem (2.7). In each of the above cases, the error is computed between the numerical approximation and the expected value solution formula on the interval $[-5, 5]$.

For each choice of λ and D^+ above, the error is computed between the stochastic numerical approximation and the expected value solution formula at specific points in space: $\{-1.5, 0, 2.5\}$. To reduce the computational time, the largest stable time step was used, however the computations each involved over ten million sample paths. The absolute value of the error is plotted versus $dt := h_n$ on a log-log plot in Figure 2 demonstrating between zero and half order accuracy in each case (note guide lines in each plot), as predicted by Theorem 6.

6. Conclusions

Diffusion problems involving discontinuities in the diffusion coefficient and interface conditions arise naturally as physical/biological models and are known to lead to interesting and often unexpected phenomena [3, 4, 5, 6, 7, 8]. As demonstrated in the present paper, the theoretical and/or numerical and computational analysis is well-aided by combining equivalent PDE and SDE versions of the phenomena. In this regard, we have constructed a stochastic Euler-Maruyama numerical method for the SDE formulation of a discontinuous diffusion problem. Our model involves a one parameter family of interface conditions coupled to a diffusion equation with discontinuous diffusion coefficient in one spatial dimension. A key idea involves a reformulation of the deterministic PDE and the stochastic SDE formulation of the diffusion problem using a

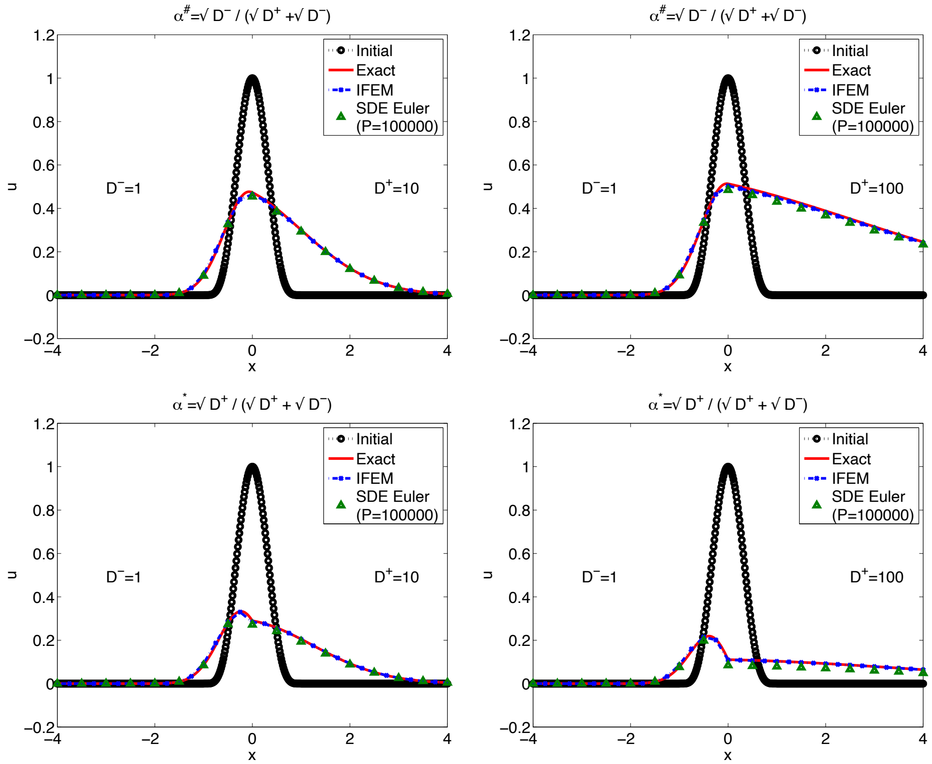

Figure 1: Initial and computed solution of (5.1) at $t = 0.2$ using IFEM method, the SDE-Euler method and the expected value solution formula from [14], for various combinations of D^+ and λ values.

change of variables, which then allows the numerical discretization methods to be developed in a natural way. We have proved the convergence and obtained the convergence rate for the Euler-Maruyama numerical method under mild assumptions. Finally, the rates of convergence of our Euler method were verified by numerical examples and compared to other approaches available in the literature for the discretization of discontinuous diffusion problems. Our formulation of an equivalent SDE model and its numerical discretization is applicable to a wide variety of interface conditions used in disparate applications spanning ecology, hydrology, astrophysics, finance and physical oceanography. Our work in this paper adds significantly to the existing literature of SDEs and their numerical discretization for diffusion problems with discontinuous coefficients across interfaces.

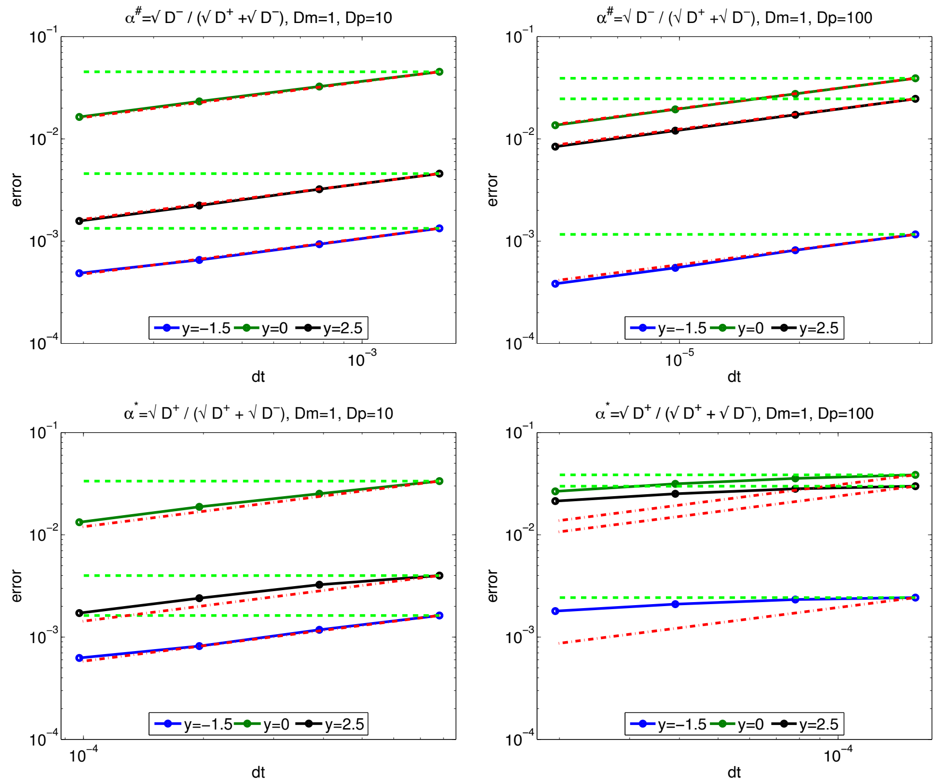

Figure 2: Error for the SDE-BE method demonstrating half order convergence (the green and red lines indicate the zeroth and half order reference lines, respectively).

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Appendix A. Smooth First-Passage Densities for One Dimensional Diffusions

In this section we provide some properties of the first passage time densities of one dimensional uniformly elliptic diffusion processes which imply the estimates for the density $r_0^x(s)$ of the first passage time before time T at point 0 of the process $Y^{(\alpha)}$. The following Lemma is a combination of Theorem A.1 and Lemma A.5 in [30].

Lemma 10. *Let γ and μ be real valued functions such that $\gamma \in C_b^{k+2}(\mathbb{R})$ and $\mu \in C_b^{k+1}(\mathbb{R})$ for some non-negative integer k. Suppose that there is a positive constant λ such that $\gamma(x) > \lambda$ for all x and $Z(t)$ satisfies*

$$Z(t) = Z_0 + \int_0^t \mu(Z(s))ds + \int_0^t \gamma(Z(s))dB(s).$$

a, Denote $\tau_0(Z) = \inf\{s > 0 : Z_s = 0\}$. If $T > 0$ and $x \neq 0$ then under $\mathbb{P}^x$, the first passage time of $Z(t)$ at point 0 before time T, $\tau_0(Z) \wedge T$, has a smooth density $r_0^x(s)$ which is of class $C^k\big((0,T] \times (-\infty, 0)\big)$.
b, In addition, if $k \geq 2$ then for all $0 \leq \alpha < 1$ there exists a constant C such that

$$\int_0^t \frac{1}{s^\alpha} r_0^x(t-s)ds \leq \frac{C}{t^\alpha} \quad \text{for all} \;\; 0 \leq t \leq T \;\text{ and } x \neq 0.$$

We also have the following estimate from [30] (See Lemma A.6).

Lemma 11. *There exists a positive constant $\tilde{C}$ such that for $0 \leq \alpha \leq 1$ and any function H bounded on $[0,T]$, continuously differentiable on $(0,T]$ satisfying*

$$H(0) = 0, \quad |H'(s)| \leq \frac{C_H}{s^\alpha} \;\forall s \in (0,T]$$

we have

$$\Big|\frac{\partial}{\partial x}\int_0^t r_0^x(t-s)H(s)ds\Big| \leq C_H\tilde{C}, \quad \Big|\frac{\partial^2}{\partial x^2}\int_0^t r_0^x(t-s)H(s)ds\Big| \leq C_H\tilde{C}\Big(1+\frac{1}{t^\alpha}\Big),$$

for all $t \in (0,T]$ and $x \neq 0$.