BOUNDARY PRESERVING SEMIANALYTIC NUMERICAL ALGORITHMS FOR STOCHASTIC DIFFERENTIAL EQUATIONS[*]

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Abstract. Construction of splitting-step methods and properties of related nonnegativity and boundary preserving semianalytic numerical algorithms for solving stochastic differential equations (SDEs) of Itô type are discussed. As the crucial assumption, we oppose conditions such that one can decompose the original system of SDEs into subsystems for which one knows either the exact solution or its conditional transition probability. We present convergence proofs for a newly designed splitting-step algorithm and simulation studies for numerous well-known numerical examples ranging from stochastic dynamics occurring in asset pricing in mathematical finance (Cox–Ingersoll–Ross (CIR) and constant elasticity of variance (CEV) models) to measure-valued diffusion and super-Brownian motion (stochastic PDEs (SPDEs)) as met in biology and physics.

Key words. stochastic differential equations, absorbing boundary, numerical methods, super-Brownian motion, splitting-step algorithm, convergence, nonnegativity, simulation

AMS subject classifications. 65C30, 60H10, 60H15

DOI. 10.1137/05063725X

1. Introduction and examples. Stochastic differential equations (SDEs) are fundamental to describe and understand random phenomena in different areas of physics, engineering, economics, etc. Particularly, they serve as models for price fluctuations as in the famous Black–Scholes option pricing model, description of erratic movements of particles as in the Langevin equation, or spatial processes like the super-Brownian motion (sBm). In most cases, explicit solutions of SDEs are very difficult to obtain and numerical approximations need to be exploited. In fact a wealth of methods for numerically integrating SDEs are known and tested [27, 28, 31, 40, 41, 42, 43, 46].

In some practical applications autonomous Itô-type SDEs of the form

$$(1.1) \qquad dX(t) = f(X(t))\,dt + \sigma(X(t))\,dW(t), \quad X(0) = X_0 \in \mathcal{D}$$

are well defined only with certain boundary conditions at the boundaries of the domain $\mathcal{D}$ in which $X(t)$ lives for all t (almost surely). These boundary conditions could be additionally imposed or naturally inherent in (1.1). For example, if $X(t)$ is the price of a stock and (1.1) gives its time-evolution, then $\mathcal{D} = [0, \infty)$, where $X(t) = 0$ implies an absorbing or reflecting state. Or, if $X(t)$ models the number of certain species in a noisy environment, then $\mathcal{D} = [0, K]$, where K is an attracting carrying capacity of the environment. When the boundaries are unattainable in finite time, conditions at the boundary are not needed to define the problem (1.1). This is the case of *natural boundaries*, according to Feller's classification [14, 15, 16, 17].

The aim of this paper is to present an alternative strategy, based on *splitting-step methods* to numerically integrate SDEs (1.1) subject to natural boundary conditions,

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that guarantees both that the numerical solutions live in the domain $\mathcal{D}$ and that the character of the boundary is preserved. Our analysis focuses mainly on the case of naturally inherent boundaries in the exact solution and its numerical approximation. It is important to stress that, although our method relies heavily on the knowledge of the exact solution of related stochastic processes and thus its validity is not strictly general, a wide variety of paramount problems known in the literature ranging from finance to physics or biology can be treated efficiently. Moreover, the consistency of this new method shall be mathematically justified by two convergence theorems, namely, one for sufficiently smooth Lipschitzian coefficients of involved SDEs (Theorem 3.1 in the main text) and another one (Theorem C.1 in the appendix) based on the variation-of-parameters formula (VOP). By those theorems we are going to establish the convergence rates which are equal to or higher than standard methods (e.g., 1.0 for global L^2-convergence in contrast to the rate 0.5 of Euler-type methods). Finally, the computational method is complemented with a very fast algorithm to sample an important class of conditional transition probabilities found in important problems.

The standard (unrestricted) Brownian motion on $\mathbb{R}$ is the most obvious example of natural boundaries at infinity. Reasonable population models in ecology, interest rates, or asset prices in finance possess the natural boundary at 0 (i.e., nonnegativity). The situation is different when the solution of (1.1) attains the boundaries in finite time. In this case, boundary conditions can be naturally inherent or imposed such as *absorbing / killing* or *reflecting boundaries*—for example, the Brownian motion on $\mathbb{R}^+$ for which a boundary condition at $x = 0$ needs to be specified to completely define its solution.

The problem of how to handle boundary conditions also appears in the numerical approximations of (1.1). Naturally inherent boundary conditions do need to be incorporated in the construction of its numerical approximations too. In fact, standard numerical methods such as Euler methods may fail to meet these boundary conditions; see [39]. This is also true for higher order converging Taylor-type methods [27, 28, 41]. Numerical time-discretizations face two kinds of different (though related) problems when a boundary condition is specified. The first one is to restrict the values of the numerical approximations to live within the domain $\mathcal{D}$; second, they also have to preserve the character of the boundary (natural, reflecting, absorbing, etc.).

There are several methods of numerically approximating the solutions of (1.1) when boundary conditions are imposed at the boundaries of $\mathcal{D}$. In the case of natural boundaries (related to Neumann boundary conditions in approximations of parabolic PDEs), methods involving projection techniques [29], penalty methods [26, 38], or symmetrized schemes [1] have been proved successful. For absorbing boundary conditions (related to Dirichlet boundary conditions in PDEs), the strategies involving direct Euler schemes [13, 19, 20] or exploiting the well-known Feynman–Kac representation formula [3] are applied. Finally, in the case of natural boundaries, i.e., when the diffusion does not reach the boundary, balanced implicit methods (see [32, 40, 41]), balanced Milstein methods [25], or composition methods based on Lie algebra techniques [33] are efficient methods of incorporating boundary restrictions. In other specific cases, numerical approximations of (1.1) in $\mathcal{D}$ are obtained by using standard methods and modifying the equation whenever the approximation lies outside $\mathcal{D}$ (e.g., [21, 8]).

In contrast to all forementioned citations, we shall follow a rather different, semi-analytic numerical approach to systems of SDEs (1.1). Our approach heavily relies on the exploitation of the specific structure of the original system (1.1) which al-

lows a natural splitting into explicitly known parts of the underlying dynamics with well-known boundary behavior and the remaining parts to be treated numerically with naturally incorporated boundary behavior (or even without restrictions). The method is especially efficient at approximating solutions of SDEs (1.1) where boundary conditions are naturally inherent. To exemplify the class of problems and its numerical approximations, consider the well-known square-root diffusion of Cox, Ingersoll, and Ross [5],

$$(1.2) \qquad dX(t) = [a + bX(t)] \, dt + \sigma \sqrt{X(t)} \, dW(t), \quad X(0) = x_0 \geq 0$$

with real parameters $a \geq 0$, $b \in \mathbb{R}$, and $\sigma > 0$, which is widely used for interest rate modeling or as an alternative to geometric Brownian motion occurring in the Black–Scholes model of dynamic asset pricing in mathematical finance. It is well known that the (strong) solution of (1.2) is unique, preserves the nonnegativity of the initial data, and has different boundary behavior at $X(t) = 0$ depending on the values of a and σ (see section 5.1). For the real-valued numerical implementation of the $\sqrt{X(t)}$-term, the nonnegativity of numerical approximations of (1.2) is of special importance. In fact, the nonnegativity (and hence the exclusive real-valued numerical evaluation) can be easily achieved in numerical approximations by means of balanced implicit methods (see [32, 40, 41]), balanced Milstein methods [25], and composition methods based on Lie algebra techniques [33]. However, the latter-mentioned or other methods may fail to incorporate the right boundary properties in the numerical paths. Other methods, while converging in the limit $\Delta t \to 0$, do not even conserve the nonnegativity of the solution like that of the straightforward fixing by taking $\sqrt{|X(t)|}$ instead of the diffusion term $\sqrt{X(t)}$ in (1.2) (as done in [21] or [8]). Recall that convergence as $\Delta t \to 0$ is an asymptotic property, but nonnegativity or boundary preserving property is more of qualitative nature and important from the point of view of adequate modeling interpretation (while using nonzero step sizes as in computational practice).

The following sections are structured as follows. We introduce and discuss the general splitting-step algorithm in section 2. Section 3 reports on a general convergence theorem and its mathematical proof. Several numerical experiments in sections 4–6 strongly support the suggested algorithm and results from previous sections by ordinary SDEs. In section 4 we present some simple models and related experiments. Section 5 is devoted to the simulation of processes as often met in dynamic asset pricing in mathematical finance. In section 6 we mention some applications to measure-valued diffusions and reaction-diffusion equations demonstrating the potential range of the splitting-step algorithm for numerical treatment of random PDEs. Section 7 concludes with some supplemental remarks. Eventually, there are three small appendices on aspects of random number generation and strong path approximations and on a convergence theorem based on the VOP with an illustrative example.

2. Splitting-step algorithm. The general structure of a splitting-step algorithm, which is based on the idea in [37] (see also [34, 10]), is as follows. Suppose that the more general equation which is to be integrated is of the form

$$(2.1) \qquad dX(t) = [\alpha(X(t), t) + \beta(X(t), t)] \, dt + \sigma(X(t), t) \, dW(t).$$

We then decompose the above equation into the two equations

$$(2.2) \qquad dX_1(t) = \beta(X_1(t), t) \, dt + \sigma(X_1(t), t) \, dW(t),$$
$$(2.3) \qquad dX_2(t) = \alpha(X_2(t), t) \, dt,$$

where the splitting is done assuming that we know the exact strong solution for $X_1(t)$ or the conditional probability $\mathcal{P}[X_1(t)|X_1(0)]$. Thus, we can approximate the solution of (2.1) by a stochastic process Y_t along time intervals $[t, t + \Delta t]$ using the following two-step algorithm for each Δt, which we call the *splitting-step algorithm*:

Step 1. Knowing the value of Y_t we obtain an intermediate value $\tilde{Y}_t$ which is obtained through the exact integration of (2.2) and $\tilde{Y}_t = X_1(t + \Delta t)$ and with initial condition $X_1(t) = Y_t$.

Step 2. Then $\tilde{Y}_t$ is used as the initial condition for (2.3) which is now integrated using any converging deterministic numerical algorithm to get $\tilde{X}_2$ (at least of deterministic order 1). Then $Y_{t+\Delta t} = \tilde{X}_2(t + \Delta t)$.

As said before, we *assume* that either the analytic expression of the exact strong solution of X_1 governed by (2.2) or its conditional transition probabilities $\mathcal{P}[X_1(t)|X_1(0)]$ are explicitly known. Thus, the advantage of this splitting-step technique for SDEs subject to boundary conditions is that if (2.2) is simple enough and we know the solution X_1 of (2.1), then the stochastic part of the problem can be handled correctly. For example, for the case $\beta(X_1, t) = 0$ and $\sigma(X_1, t) = \sqrt{X_1}$, it is known that the conditional probability distribution is given by

$$(2.4) \qquad \mathcal{P}[X_1(t)|X_1(0)] = \frac{2}{t} \left(\frac{X_1(0)}{X_1(t)} \right)^{1/2} I_1 \left(\frac{4}{t} \sqrt{X_1(t)X_1(0)} \right) e^{-\frac{2}{t}[X_1(t)+X_1(0)]}$$
$$+ e^{-\frac{4}{t}X_1(0)} \delta(X_1(t)),$$

where I_1 is the modified Bessel function and $\delta(x)$ is the Dirac delta function.

This cdf can be sampled using the rejection or inverse methods but this is computationally expensive. However, we introduce here a very simple method [34] (see also [2]) for obtaining $X_1(t)$ by noting that the variable $Z(t) = \frac{4}{t} X_1(t)$ has a probability distribution given by the noncentral χ^2-distribution, that is,

$$(2.5) \qquad \mathcal{P}[Z|Z_0] = \sum_{j=1}^{\infty} \frac{(\lambda/2)^j e^{-\lambda/2}}{j!} \mathcal{P}_{\chi_{2j}^2}(Z) + e^{-\lambda/2} \delta(Z),$$

where $\lambda = \frac{4}{t} Z_0$ and $\mathcal{P}_{\chi_{2j}^2}(X)$ is the χ^2-pdf with $2j$ degrees of freedom. Equation (2.5) reveals that the probability distribution for Z is a linear combination of χ^2-pdfs with Poisson weights. This fact can be exploited to generate $X_1(t)$ efficiently. If we choose K from a Poisson distribution with mean $\lambda/2$, then

$$(2.6) \qquad X_1(t) = \frac{1}{2k} \begin{cases} 0 & \text{if } K = 0, \\ \sum_{i=1}^{2K} z_i^2 & \text{if } K \neq 0, \end{cases}$$

where z_i are independent Gaussian random numbers with zero mean and unit variance. Computationally, it is faster to sample the random number $\sum_{i=1}^{2K} z_i^2$ using standard algorithms for random number generation of the χ^2 distribution. Other examples of this sampling can be found in section 4 and the appendix.

The obvious advantage of the splitting algorithm is that we exploit the structure of the original equation more efficiently. For example, in the above example, we get numbers from (2.6) which are nonnegative and thus, if $\alpha(X, t)$ has nice properties, the approximated values for $X(t)$ are nonnegative, too. Such a splitting algorithm is not known from the literature to the best of our current knowledge, although the idea of

splitting is not new for dynamical systems and their numerical integration. A different kind of splitting technique has been suggested in [22]. However, their algorithm, called the split-step Euler method, is related to another subclass of splitting of SDEs and their resulting split-step algorithm is of lower order 0.5 of mean square convergence, which is restricted by their use of the (drift-implicit) backward Euler method. Their method indirectly refers to the splitting

$$dX_1(t) = [\alpha(X_1(t), t) + \beta(X_1(t), t)] \, dt,$$
$$dX_2(t) = \sigma(X_2(t), t) \, dW(t),$$

of the original system (1.1) in our set-up, where both equations for X_1 and X_2 are numerically integrated in a separated fashion. In contrast to them, by a more efficient choice of splitting, we even suggest removing stochastic integrals from numerical integration by appropriate splitting of (1.1) in order to achieve a higher order of convergence, and our technique is not restricted only to techniques of direct pathwise simulation. It may be noted that the explicit removal of stochastic integrals from numerical integration by splitting techniques is always possible and leads to converging numerical approximations with higher order under some appropriate assumptions on the diffusion coefficient σ (for example, $\sigma\sigma\prime$ has sufficiently many bounded derivatives) in $\mathbb{R}^1$. Another form of splitting has been suggested in [6]. They present an algorithm which also takes advantage of techniques of numerical integration of ODEs. However, neither [6] nor [22] discusses the issue of pathwise preservation of nonnegativity, monotonicity, and boundedness by their numerical approximation techniques.

3. A convergence theorem of splitting algorithm for nonautonomous equations. Let $C^{i,j}(\mathbb{R}^d \times [0, T])$ denote the vector space of continuous functions $f = f(x, t)$ which are i times continuously differentiable with respect to the space-coordinate $x_k \in \mathbb{R}$ ($k = 1, 2, \ldots, d$) and j times continuously differentiable with respect to time-coordinate $t \in [0, T]$. Recall that the original equation is

$$(3.1) \qquad dX(t) = [\alpha(X(t), t) + \beta(X(t), t)] \, dt + \sigma(X(t), t) \, dW(t).$$

For the proof of splitting techniques below, we refer the reader to the splitting

$$(3.2) \qquad dX_1(t) = \beta(X_1(t), t) \, dt + \sigma(X_1(t), t) \, dW(t),$$
$$(3.3) \qquad dX_2(t) = \alpha(X_2(t), t) \, dt.$$

THEOREM 3.1. *Assume that the coefficient functions $\alpha, \beta \in C^{2,1}(\mathbb{R}^d \times [0, T])$ and $\sigma \in C^{3,2}(\mathbb{R}^d \times [0, T])$ with exclusively uniformly bounded derivatives are such that*

$$\sup_{0 \le t \le T} \mathbb{E} \left[|X(t)|^2 + |\alpha(X(t), t)|^2 + |\beta(X(t), t)|^2 + |\sigma(X(t), t)|^2 \right] < +\infty$$

for a fixed, finite, nonrandom terminal time $T > 0$. Then the splitting-step algorithm with steps 1 and 2 has (global) strong and weak order 1.0 of convergence on the interval $[0, T]$ (in the worst case).

Proof. For simplicity, suppose that $d = 1$. Let

$$0 = t_0 < t_1 < \cdots < t_n < t_{n+1} < \cdots < t_N = T$$

be any nonrandom partition of the given time-interval $[0, T]$ with sufficiently small maximum step size $\Delta = \max_{i=1,2,\ldots,N} |t_i - t_{i-1}| \le 1$. Define the local pathwise error

by $\varepsilon_{n+1}^{loc} = X(t_n + \Delta_n t) - \tilde{X}(t_n + \Delta_n t)$ assuming that both exact solution X and its approximation $\tilde{X}$ have started at the same value $X(t_n)$ at time t_n. To investigate this error, apply the stochastic Taylor formula to the processes X, X_1, and X_2—an idea which originates from the Wagner–Platen expansion [47] and was popularized by [27] (more precisely speaking, this exploits the idea of an iterative application of the Itô formula). For the sake of abbreviation, we shall write z_n or z_u for all occurring coefficients or processes (not referring to partial derivatives here); hence $X_n = X(t_n)$, $\alpha_n = \alpha(X(t_n), t_n)$, $\beta_n = \beta(X(t_n), t_n)$, and $\sigma_n = \sigma(X(t_n), t_n)$, and similarly, $\alpha_u = \alpha(X(u), u)$, $\beta_u = \beta(X(u), u)$, $\sigma_u = \sigma(X(u), u)$, and so on, unless it is stated differently wherever convenient. Define the partial differential operators

$$L_0^0 f(x,t) = \frac{\partial f(x,t)}{\partial t} + [\alpha(x,t) + \beta(x,t)]\frac{\partial f(x,t)}{\partial x} + \frac{1}{2}[\sigma(x,t)]^2\frac{\partial^2 f(x,t)}{\partial x^2},$$

$$L_0^1 f(x,t) = \sigma(x,t)\frac{\partial f(x,t)}{\partial x}, \quad L_1^1 f(x,t) = L_0^1 f(x,t),$$

$$L_1^0 f(x,t) = \frac{\partial f(x,t)}{\partial t} + \beta(x,t)\frac{\partial f(x,t)}{\partial x} + \frac{1}{2}[\sigma(x,t)]^2\frac{\partial^2 f(x,t)}{\partial x^2},$$

$$L_2^0 f(x,t) = \frac{\partial f(x,t)}{\partial t} + \alpha(x,t)\frac{\partial f(x,t)}{\partial x},$$

where L_i^0 is mapping from $C^{2,1}(\mathbb{R}^d \times [0,T])$ to $C^{0,0}(\mathbb{R}^d \times [0,T])$ and L_i^1 from $C^{1,0}(\mathbb{R}^d \times [0,T])$ to $C^{0,0}(\mathbb{R}^d \times [0,T])$ for $i = 1, 2$, and L_2^0 from $C^{1,1}(\mathbb{R}^d \times [0,T])$ to $C^{0,0}(\mathbb{R}^d \times [0,T])$. First, apply Taylor-type approximations to the solutions of (3.1) to obtain

$$X_{n+1} = X_n + \int_{t_n}^{t_{n+1}} [\alpha(X(s), s) + \beta(X(s), s)]\, ds + \int_{t_n}^{t_{n+1}} \sigma(X(s), s)\, dW(s)$$

$$= X_n + [\alpha_n + \beta_n]\Delta_n t + \sigma_n \Delta_n W$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0(\alpha_u + \beta_u)\, du\, ds + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^1(\alpha_u + \beta_u)\, dW(u)\, ds$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0 \sigma_u\, du\, dW(s) + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^1 \sigma_u\, dW(u)\, dW(s)$$

(3.4) $$= X_n + [\alpha_n + \beta_n]\Delta_n t + \sigma_n \Delta_n W + \frac{1}{2}L_0^1 \sigma_n[(\Delta_n W)^2 - \Delta_n t] + R_{0,n}$$

with the remainder term

$$R_{0,n} = \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0(\alpha_u + \beta_u)\, du\, ds + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^1(\alpha_u + \beta_u)\, dW(u)\, ds$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0 \sigma_u\, du\, dW(s) + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_0^0 L_0^1 \sigma_v\, dv\, dW(u)\, dW(s)$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_0^1 L_0^1 \sigma_v\, dW(v)\, dW(u)\, dW(s).$$

Now, we compare (3.4) with what we get from the expansion of the splitting method. In the latter case, by application of the Wagner–Platen expansion [47] again, we arrive at

$$X_{1,n+1} = X_n + \int_{t_n}^{t_{n+1}} \beta(X_1(s), s)\, ds + \int_{t_n}^{t_{n+1}} \sigma(X_1(s), s)\, dW(s)$$

$$= X_n + \beta_n \Delta_n t + \sigma_n \Delta_n W$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0 \beta_u \, du \, ds + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^1 \beta_u \, dW(u) \, ds$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0 \sigma_u \, du \, dW(s) + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^1 \sigma_u \, dW(u) \, dW(s)$$

$$(3.5) \qquad = X_n + \beta_n \Delta_n t + \sigma_n \Delta_n W + \frac{1}{2} L_1^1 \sigma_n [(\Delta_n W)^2 - \Delta_n t] + R_{1,n}$$

with the remainder term

$$R_{1,n} = \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0 \beta_u \, du \, ds + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^1 \beta_u \, dW(u) \, ds$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0 \sigma_u \, du \, dW(s) + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_1^0 L_1^1 \sigma_v \, dv \, dW(u) \, dW(s)$$

$$+ \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_1^1 L_1^1 \sigma_v \, dv \, dW(u) \, dW(s).$$

Here, the coefficients β and σ involved in the above integrals are evaluated at the arguments $(X_1(u), u)$ and $(X_1(v), v)$, respectively. Similarly, by deterministic Taylor expansion for the local approximation of (3.3) in the framework of the splitting method, one gets

$$(3.6) \quad X_{2,n+1} = X_{1,n+1} + \int_{t_n}^{t_{n+1}} \alpha(X_2(s), s) \, ds = X_{1,n+1} + \alpha(X_{1,n+1}, t_n) \Delta_n t + R_{2,n}$$

with the remainder term

$$R_{2,n} = \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_2^0 \alpha_u \, du \, ds$$

$$= \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \left[\frac{\partial \alpha(X_2(u), u)}{\partial u} + \alpha(X_2(u), u) \frac{\partial \alpha(X_2(u), u)}{\partial x} \right] du \, ds.$$

Here, the coefficients α involved in the above integrals are evaluated at the arguments $(X_2(u), u)$. An expansion of $\alpha(X_{1,n+1}, t_n)$ with respect to space-variable x gives

$$(3.7) \quad \alpha(X_{1,n+1}, t_n) = \alpha_n + \int_{t_n}^{t_{n+1}} L_1^0 \alpha(X_1(s), s) \, ds + \int_{t_n}^{t_{n+1}} L_1^1 \alpha(X_1(s), s) \, dW(s).$$

Now, plug expansions (3.7) and (3.5) into (3.6) in order to obtain

$$(3.8) \qquad X_{2,n+1} = X_n + [\alpha_n + \beta_n] \Delta_n t + \sigma_n \Delta_n W + \frac{1}{2} L_1^1 \sigma_n [(\Delta_n W)^2 - \Delta_n t] + R_{3,n}$$

with the remainder term

$$R_{3,n} = R_{1,n} + R_{2,n} + \left[\int_{t_n}^{t_{n+1}} L_1^0 \alpha_s \, ds + \int_{t_n}^{t_{n+1}} L_1^1 \alpha_s \, dW(s) \right] \Delta_n t.$$

Consequently, the local pathwise error $\varepsilon_{n+1}^{loc} = X_{n+1} - X_{2,n+1}$ can be represented by

$$
\begin{aligned}
\varepsilon_{n+1}^{loc} &= X_{n+1} - X_{2,n+1} = R_{0,n} - R_{3,n} \\
&= \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0(\alpha_u + \beta_u)\, du\, ds + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^1(\alpha_u + \beta_u)\, dW(u)\, ds \\
&\quad + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_0^0\sigma_u\, du\, dW(s) + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_0^0 L_0^1\sigma_v\, dv\, dW(u)\, dW(s) \\
&\quad + \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_0^1 L_0^1\sigma_v\, dW(v)\, dW(u)\, dW(s) \\
&\quad - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0\beta_u\, du\, ds - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^1\beta_u\, dW(u)\, ds \\
&\quad - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_1^0\sigma_u\, du\, dW(s) - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_1^0 L_1^1\sigma_v\, dv\, dW(u)\, dW(s) \\
&\quad - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{u} L_1^1 L_1^1\sigma_v\, dv\, dW(u)\, dW(s) - \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} L_2^0\alpha_u\, du\, ds \\
&\quad - \left[\int_{t_n}^{t_{n+1}} L_1^0\alpha_s\, ds + \int_{t_n}^{t_{n+1}} L_1^1\alpha_s\, dW(s) \right] \Delta_n t.
\end{aligned}
$$

(3.9)

Now recall that α, β, σ have exclusively uniformly bounded derivatives and their second moments along the solution of (3.1) are bounded on $[0, T]$. Therefore, all operators L_i^j applied to coefficients α, β, and σ have images with uniformly bounded second moments. This implies that $\mathbb{E}\,\varepsilon_n^{loc} = \mathcal{O}([\Delta_n t]^2)$ and $\mathbb{E}\,(\varepsilon_n^{loc} - \mathbb{E}\,\varepsilon_n^{loc})^2 = \mathcal{O}([\Delta_n t]^3)$. For mean square convergence, it remains to apply fairly general convergence theorems as known from [31, 42, 43] with local rates $r_1 = 2$ and $r_2 = 1.5$ in order to conclude the global strong (i.e., in the L^2-sense) convergence order $r = 1.0$. More precisely, we have

$$
\max_{n=0,1,\dots,N} \left(\mathbb{E}\,|X(t_n) - \tilde{X}(t_n)|^2 \right)^{1/2} = \mathcal{O}(\Delta)
$$

provided that the initial errors $\mathbb{E}\,|X(0) - \tilde{X}(0)|^2 = \mathcal{O}(\Delta^2)$ started at L^2-integrable initial values which are independent of the σ-algebra generated by the underlying Wiener process W. Eventually, the global order $r_w = 1.0$ of weak convergence with respect to smooth, polynomially bounded test functions is rather obvious from the fact that the local weak rate $r_w = 2.0$ (exploiting standard techniques known from [17] and [31] on weak convergence analysis). Consequently, the splitting-step algorithm has the claimed convergence orders, and the proof is complete. □

4. First illustrative numerical experiments. In this section we give several illustrative and important examples of applying our new stochastic numerical schemes to SDEs and test the rate of convergence obtained in section 3.

4.1. Using the transition probability. Consider the splitting-step method applied to the SDE

(4.1) $$ dX(t) = (1 + X(t))\, dt + 2\sqrt{X(t)}\, dW(t) $$

with $\alpha(X, t) = 1 + X$, $\beta(X, t) = 0$, and $\sigma(X, t) = 2\sqrt{X}$. The conditional transition probability for the stochastic part of the splitting algorithm is sampled using (2.6).
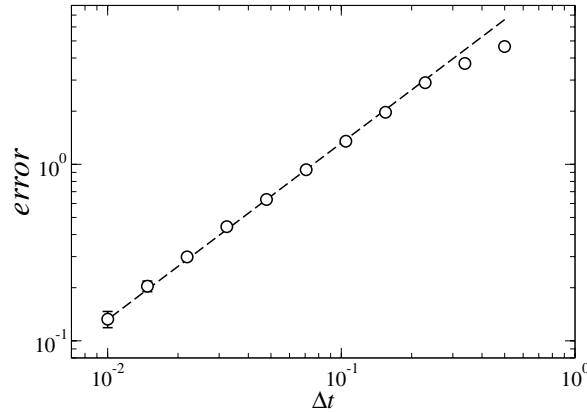
FIG. 4.1. *Absolute value of the error* (4.3) *as a function of* Δt *for* $t = 1.0$ *and* $X(0) = 1$ *obtained using the splitting-step algorithm. The dashed line is proportional to* Δt.

The conditional mean value is given by

$$(4.2) \qquad \mathbb{E}\left(X(t)|X(0) = x_0\right) = (x_0 + 1)e^t - 1$$

for any nonrandom value $x_0 \geq 0$. In Figure 4.1 the error

$$(4.3) \qquad \varepsilon_1 = |\mathbb{E}\,\tilde{X}(t) - [(x_{0-1})e^t - 1]|$$

versus the decreasing uniform step size Δt is depicted, where $\tilde{X}(t)$ is the solution obtained through the numerical approximation. Figure 4.1 shows statistical numerical evidence that the method has weak order 1.0 while using constant step sizes Δt.

4.2. Using the exact solution. Consider the splitting-step algorithm applied to

$$(4.4) \qquad dX(t) = \left(X(t) - [X(t)]^3\right) dt + X(t)\, dW(t),$$

which is called the stochastic planar Ginzburg–Landau equation. In this case we take advantage of the known exact solution for the linear part of this equation which is
$$(4.5)$$
$$dX_1(t) = X_1(t)\, dt + X_1(t)\, dW(t) \Rightarrow X_1(t) = X_1(s) \exp\left((t - s)/2 + W(t) - W(s)\right).$$

To integrate the second part of the split system

$$(4.6) \qquad dX_2(t) = -[X_2(t)]^3\, dt$$

we use a partial-implicit nonstandard technique which is a nonnegativity preserving one[1] given by

$$(4.7) \qquad X_2(t + \Delta t) = X_2(t) - \frac{\Delta t}{2} X_2^2(t)[X_2(t) + X_2(t + \Delta t)].$$

_____

[1]This is true if current step size $\Delta_n t$ is chosen such that $[X_2(t_n)]^2 \Delta_n t < 2$.
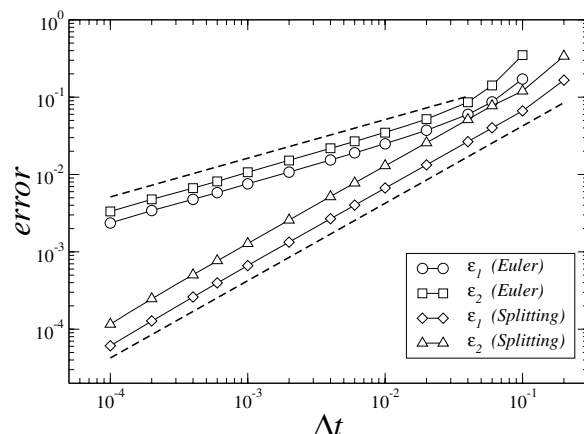
Fig. 4.2. *Value of the error* (4.8) *as a function of* Δt *for* $t = 5.0$ *and* $X(0) = 1.0$ *using the splitting-step and Euler algorithms. Dashed lines are the power laws* Δt *and* $\sqrt{\Delta t}$.

Our results for the strong error

$$(4.8) \qquad \varepsilon_k(t) = \left(\mathbb{E}\,|X(t) - \tilde{X}(t)|^k\right)^{1/k}$$

are shown in Figure 4.2 for $k = 1, 2$ and compared to the Euler algorithm for the same equation. Obviously, our results indicate that our proposed splitting method indeed is of strong order 1.0 while using constant step sizes Δt.

5. Stochastic models in finance. In this section we apply the splitting-step method to some fundamental models in mathematical finance. This application will also serve to introduce other algorithmically simple samplings of conditional probability transitions as for the $\sqrt{X_1(t)}$ case shown in the introduction.

5.1. Interest rate model of Cox, Ingersoll, and Ross. An interesting example in which the splitting-step scheme is particularly efficient is the Cox–Ingersoll–Ross (CIR) model [5] for stochastic interest rates

$$(5.1) \qquad dX(t) = [a + bX(t)]\,dt + \sigma\sqrt{X(t)}\,dW(t), \quad X(0) = x_0 \geq 0$$

with real parameters $a \geq 0$, $b \in \mathbb{R}$, and $\sigma > 0$. As stated in the introduction, strong solutions of (5.1) are nonnegative. However, depending on the specific values of parameters a, b, and σ, distinct behavior at the boundary is possible.

- If $a \geq \sigma^2/2$, then the solution is always positive. $X(t) > 0$ if $x_0 > 0$, because the boundary $X(t) = 0$ becomes unattainable.
- If $a < \sigma^2/2$, there are infinite many values of $t > 0$ for which $X(t) = 0$. The boundary becomes attainable, but it is (instantaneously) reflecting. That is, when a sample path reaches 0, then it returns immediately to the interior of the state space in a reflecting manner.

The exact transition density for the CIR process is known, but its sampling can be difficult depending on the parameters a, b, and σ. Here we may exploit the simplest splitting which appropriately reflects the boundary behavior of the CIR process by SDEs

$$(5.2) \qquad dX_1(t) = a\,dt + \sigma\sqrt{X_1(t)}\,dW(t),$$
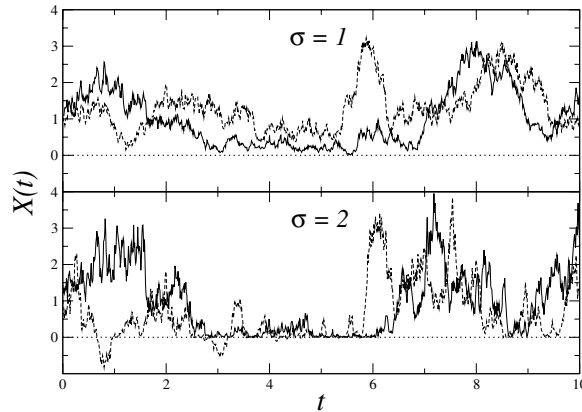
$$(5.3) \qquad dX_2(t) = bX_2(t)\,dt,$$

FIG. 5.1. *Numerical approximation of the CIR process* (5.1) *using the splitting-step method* (5.2) *(solid line) and the method proposed in* [21] *(dashed line) with* $a = b = 1$, $\Delta t = 10^{-2}$, $X(0) = 1$, *and different values of* σ: *The upper panel shows the case* $a \geq \sigma^2/2$ *where the boundary at zero becomes unattainable, while the lower panel is for* $a < \sigma^2/2$. *The splitting-step numerical approximation reproduces the attainability of the boundary condition while preserving the nonnegativity of the solution of* (5.1), *whereas the method in* [21] *has trajectories which take negative values for* $X(t)$.

which can be easily inferred by noting that the boundary behavior does not depend on the parameter b. To integrate the first step in the splitting-step system (5.2)–(5.3) we note that the process defined by (5.2) represents an a-dimensional Bessel process [17]. Its transition density $\mathcal{P}[X_1(t + \Delta t)|X_1(t)]$ can be written in terms of a noncentral χ^2 distribution and, in particular, we have

$$(5.4) \qquad X_1(t + \Delta t) = \frac{\sigma^2 \Delta t}{4} \chi'^2_d(\lambda),$$

where

$$(5.5) \qquad \lambda = \frac{4X_1(t)}{\sigma^2 \Delta t}, \qquad d = \frac{4a}{\sigma^2},$$

and $\chi'^2_d(\lambda)$ random numbers can be sampled using the algorithms in the appendix. The last part of the splitting-step scheme (5.3) can be integrated exactly or using numerical approximations. In our case we use deterministic Euler approximations where nonnegativity is preserved if Δt is small enough. Our simulations for the CIR process are shown in Figure 5.1. The boundary behavior for different values of a and σ is reproduced and, at the same time, nonnegativity is conserved. Note that other usual integration strategies such as that of [21] eventually produce negative values for $X(t)$ (for finite Δt) which lack any possible interpretation in the context of finance and could induce severe errors in option valuation.

5.2. Constant elasticity volatility models. Another important stochastic process in finance is the constant elasticity of variance (CEV) diffusion to model asset prices. This process, first introduced to finance by Cox [4], is capable of reproducing the volatility smile observed in the empirical data unlike other standard price models such as the Black–Scholes–Merton geometric Brownian motion. The process is defined as

$$(5.6) \qquad dX(t) = \mu X(t)\, dt + \sigma X(t)^\gamma\, dW(t), \quad X(0) = x_0.$$

The CEV model includes the geometric Brownian model of Black, Scholes, and Merton ($\gamma = 1$) and the square-root model of Cox and Ross ($\gamma = 1/2$). Contrary to the Black–Scholes–Merton model, the CEV model incorporates a variance adjustment that causes the absolute level of the variance to decline as the stock price rises and to rise as the stock price declines, as seen empirically in most equity and interest rate volatilities.

For our purposes, the CEV model encompasses most of the boundary conditions we can implement at $X(0) = 0$. Depending on γ, the boundary $X(0) = 0$ is the following:

- a *natural boundary* for $\gamma \geq 1$, which means that boundary is unattainable in finite time;
- an *exit or absorbing boundary* for $1/2 \leq \gamma < 1$; i.e., $X(t)$ reaches zero with finite probability in finite time and gets absorbed at it;
- a *regular boundary* for $\gamma < 1/2$. Now the boundary can be reached in finite time, and we need to specify a boundary condition at $X(0) = 0$. Typical choices are reflecting or absorbing ones.

The transition density for the CEV process is known for general values of γ and μ (see [4]). However, due to the fact that the boundary behavior of $X(t)$ does not depend on μ, we propose here the following splitting-step system:

$$(5.7) \qquad\qquad\qquad dX_1 = \sigma X_1^\gamma \, dW(t),$$

$$(5.8) \qquad\qquad\qquad dX_2 = \mu X_2 \, dt.$$

The classification of the boundary $X_1(t) = 0$ for (5.7) is the same as for (5.6). We discuss now the sampling of the transition density for each value of γ.[2]

5.2.1. $\gamma > 1$, natural boundary. In this case $X_1(t) = 0$ is unattainable and its probability transition density is given by

$$(5.9) \qquad \mathcal{P}[x_t|x_0] = \frac{x_t^{1/2-2\gamma} x_0^{1/2}}{\sigma^2(\gamma - 1)} \exp\left[-\frac{x_0^{2(1-\gamma)} + x_t^{2(1-\gamma)}}{2\sigma^2(1-\gamma)^2 t}\right] I_{\frac{1}{2(\gamma-1)}}\left[\frac{x_0^{1-\gamma} x_t^{1-\gamma}}{\sigma^2(1-\gamma)^2 t}\right].$$

To sample this distribution, we can consider the relationship between the CEV and the CIR processes. Since $X_1(t) = 0$ is not accessible, we can make the change of variables $Y_1 = X_1^{2(1-\gamma)}/[4(\gamma-1)^2\sigma^2]$ to find that $dY_1 = \lambda \, dt + \sqrt{Y_1} \, dW(t)$ where $\lambda = (1 - 2\gamma)/[4(1-\gamma)]$. Thus Y_1 is a Bessel process which can be sampled using the noncentral χ^2 distribution. At the end we have that

$$(5.10) \qquad X_1(t + \Delta t) = \left[(\gamma-1)^2\sigma^2\Delta t\, \chi_d'^2\left(\frac{X_1(t)^{2(1-\gamma)}}{\sigma^2(\gamma-1)^2\Delta t}\right)\right]^{\frac{1}{2(1-\gamma)}},$$

where $d = (1 - 2\gamma)/(1 - \gamma) \geq 1/2$. A typical path of the CEV process for $\gamma > 1$ is shown in Figure 5.2.

5.2.2. $1/2 \leq \gamma < 1$, absorbing boundary. In this case $X_1(t) = 0$ is an absorbing boundary. The transition probability density was found by Cox [4] and is given by

$$(5.11) \qquad \mathcal{P}[x_t|x_0] = \frac{x_t^{1/2-2\gamma} x_0^{1/2}}{\sigma^2(1 - \gamma)} \exp\left[-\frac{x_0^{2(1-\gamma)} + x_t^{2(1-\gamma)}}{2\sigma^2(1-\gamma)^2 t}\right] I_{\frac{1}{2(1-\gamma)}}\left[\frac{x_0^{1-\gamma} x_t^{1-\gamma}}{\sigma^2(1-\gamma)^2 t}\right].$$

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[2]We do not consider the case $\gamma = 1$, since this can be integrated using the strong solution (4.5).
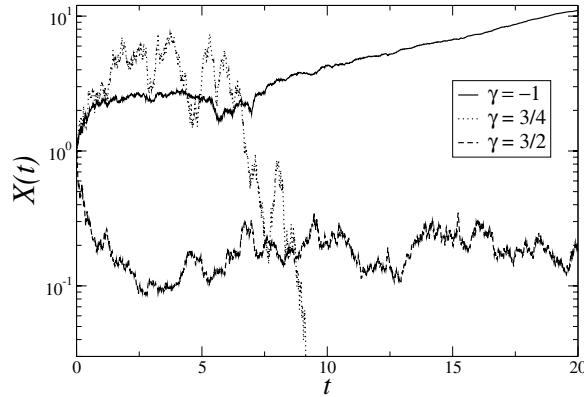
FIG. 5.2. *Numerical approximation of the CEV process* (5.6) *using the splitting-step method* (5.7)–(5.8) *for different values of* γ*. The case* $\gamma = -1$ *is the solution of* (5.6) *with reflecting boundary conditions, while the case* $\gamma = 3/4$ *gets absorbed at zero at finite time (not shown in the logarithmic scale). Parameters are* $\mu = 0.1$, $\Delta t = 10^{-2}$.

This transition probability does not integrate to one because there is a finite probability that the trajectory gets absorbed at zero given by [4]:

$$(5.12) \qquad \mathcal{P}[0|X_1(t)] = G\left(\frac{1}{2(1-\gamma)}, \frac{x_1(t)^{-2(1-\gamma)}}{2\sigma^2(1-\gamma)^2\Delta t}\right),$$

where $G(\nu, x)$ is the complementary Gamma function. For this equation, we know that trajectories of (5.7) get absorbed at zero with probability one while taking the limit $\Delta t \to \infty$. Actually, this is also the case for the solutions of (5.6) for $1/2 \leq \gamma < 1$. This is counterintuitive since the mean $\mathbb{E}[X_1(t)]$ is constant for (5.7) or grows exponentially like $x_0 e^{\mu t}$ for (5.6). This intriguing feature of (5.6) hampers the numerical simulations of this process, and in fact only exact sampling of the probability transition density (5.11) and (5.12) correctly accounts for it at finite Δt.

While similar to (5.9), the transition probability density (5.11) cannot be sampled using the relationship to the CIR process, since the solution of $dX_1 = X_1^\gamma dW(t)$ has a finite probability to be absorbed at $X_1(t) = 0$. However, using the relationship $I_n(x) = I_{-n}(x)$, $n \in \mathbb{N}$, for the modified Bessel function, we have that if $1/[2(1-\gamma)] = n$, X_1 can be sampled from a noncentral χ^2 distribution with negative (integer) number of degrees of freedom (see the appendix):

$$(5.13) \qquad X_1(t+\Delta t) = \left[(\gamma-1)^2\sigma^2\Delta t\, \chi'^2_d\left(\frac{X_1(t)^{2(1-\gamma)}}{\sigma^2(\gamma-1)^2\Delta t}\right)\right]^{\frac{1}{2(1-\gamma)}},$$

where $d = 2 - 2n = 0, -2, -4, \ldots$, and then $\gamma = 1 - 1/2n = 1/2, 3/4, 5/6, \ldots$. In Figure 5.2 we show a typical path for the CEV process for $\gamma = 3/4$ ($d = -2$) in which we see that it gets absorbed at zero for finite time.

5.2.3. $\gamma < 1/2$, **regular boundary.** Now the boundary is attainable and, contrary to the previous case, a boundary condition should be provided. If we consider the simplest cases, namely, an absorbing or reflecting boundary condition, then the transition probability density is given by

$$(5.14) \quad \mathcal{P}_\pm[x_t|x_0] = \frac{x_t^{1/2-2\gamma}x_0^{1/2}}{\sigma^2|1-\gamma|}\exp\left[-\frac{x_0^{2(1-\gamma)}+x_t^{2(1-\gamma)}}{2\sigma^2(1-\gamma)^2t}\right]I_{\pm\frac{1}{2|1-\gamma|}}\left[\frac{x_0^{1-\gamma}x_t^{1-\gamma}}{\sigma^2(1-\gamma)^2t}\right],$$

where $\mathcal{P}_+$ corresponds to the absorbing case and $\mathcal{P}_-$ to the reflecting one. In the latter case, the relationship of the CEV and CIR processes can be exploited to sample the probability distribution (5.14), with the same result as in (5.10). Simulation of the CEV process in this case is shown in Figure 5.2. However, in the absorbing case, $\mathcal{P}_-$ cannot be sampled either by using the corresponding CIR process or by using *negative dimensions* as in the previous case, since for $\gamma < 1/2$ we have that $1 < 1/[2(\gamma-1)] \leq 0$. Thus $\mathcal{P}_-$ should be sampled using rejection or transformation methods.

6. Measure valued diffusions / reaction-diffusion problems. During the last decade much attention has been devoted to stochastic spatial models of interacting and branching particles like the contact model, the voter model, and the normal and oriented percolation [45, 23, 7]. Despite its simplicity these models display interesting critical properties at high spatial dimensions and serve as universality classes for more complicated situations. While much analytical progress has been made in the study of these models, some of their properties must be understood by using numerical methods. In this respect, several efficient particle stochastic simulations have been proposed and studied. An alternative approach is to study the convergence of the particle process to a continuum measure value diffusion in which the system is described by the (stochastic) concentration of particles $u(x,t)$ at a given spatial location x. This accelerates the numerical simulations and also could help to identify the relevant dynamics at the coarse-grained dynamics. Useful representations of these measure-valued diffusions are the ones interpreted as solutions of a martingale problem in terms of stochastic PDEs (SPDEs). Despite its clear interpretation, this representation is not usually considered in numerical simulations. The reason for that is the inability of usual numerical methods to handle correctly the nonnegativity character and the Poissonian fluctuations of the concentration of particles close to $u = 0$ [34, 18]. In this respect, we will see that the splitting scheme provides a very efficient and accurate method to study these models.

6.1. Super-Brownian motion. The most simple and studied measured-valued diffusion is the super-Brownian motion (sBm). The sBm arises as the scaling limit in various critical branching systems when the interaction between them is weak, i.e., when the system is above some *critical spatial dimension* [45]. Above this critical dimension we expect a Gaussian limit and indeed the sBm is the Gaussian limit of a number of models: the voter model above two dimensions, the contact process above four dimensions, oriented percolation above four dimensions, and percolation over six dimensions.

sBm can be studied analytically by using the log-Laplace transform that maps its dynamics into a nonlinear PDE, a result due to Dynkin [12]. More general situations or particular properties of the sBm can be reached only through numerical simulations. To our knowledge there is no numerical simulation of the martingale problem of the sBm so far. In one dimension, the martingale problem of the sBm is described by the SPDE

$$(6.1) \qquad\qquad du(x,t) = \Delta u(x,t)\, dt + \sqrt{\sigma u(x,t)}\, dW(x,t),$$

where $W(x,t)$ is a Wiener sheet. It is well known that the solutions of the sBm die in finite time almost surely. Another interesting property is that the support of the solution, i.e., the set for which $u(x,t) > 0$, is compact, provided that the initial condition has a compact support. This compact support property is related to the absorbing nature of $u(x,t) = 0$. Thus it can only be recovered in the numerical
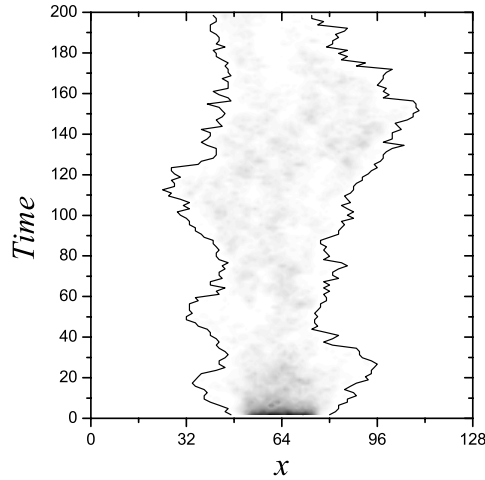
FIG. 6.1. *Realization of the sBm in one dimension. The figure shows density plots for $u(x,t)$ as a function of time with initial condition $u(x,0) = 0.1$. The solid line depicts the extremes of the support at each time. Parameters are $\Delta x = 1$, $\Delta t = 0.1$, and $\sigma = 1.0$ in an $L = 128$ lattice.*

approximations if the behavior of the boundary is incorporated. For example, the method of Gaines [18], while implementing the nonnegativity of the solutions, fails to reproduce the compact support property for the solutions of (6.1).

We use the splitting-step method for approximating the strong path solutions of (6.1). To this end we approximate the sBm by the superrandom walk on $\mathbb{Z}^d$ (see [7])

$$(6.2) \qquad du_i(t) = \Delta_i u_i(t)\, dt + \sqrt{\frac{\sigma u_i(t)}{(\Delta x)^d}}\, dW_i(t),$$

where Δ_i is the discrete Laplacian operator

$$\Delta_i u = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

in $\mathbb{Z}^d$, Δx is the lattice spacing, and $W_i(t)$ are independent Wiener processes in time t. Equation (6.2) represents a model of interacting Feller diffusions. The splitting-step algorithm in this case is based on

$$(6.3) \qquad du_i^{(1)}(t) = \sqrt{\frac{\sigma u_i^{(1)}(t)}{(\Delta x)^d}}\, dW_i(t), \quad du_i^{(2)}(t) = \Delta_i u_i^{(2)},$$

where the first step is integrated using the transition probability (2.5) and its sampling (2.6). The second equation can be integrated using standard schemes. In Figure 6.1 we observe a simulation of the sBm in one dimension. Our method not only provides an accurate description in both the strong and weak sense of the sBm; it also incorporates one of its main properties, namely, the compact support property.

In two dimensions (6.1) is not well defined, but still we can study (6.2) in the lattice $\mathbb{Z}^2$. As our simulations show (see Figure 6.2), the compact support properties of sBm in two dimensions are preserved, and we also see the clusters' formation and their disappearance at large times.
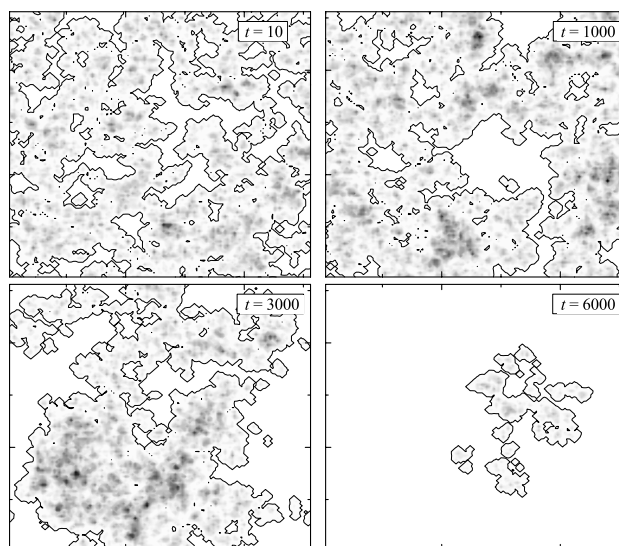
FIG. 6.2. *Strong path approximation of the sBm in two dimensions. The figures show density plots of $u(x,t)$ surrounded by the border of the support (solid line) at different times. The initial condition is $u(\vec{r},0) = 0.1$. Parameters are $\Delta x = 1$, $\Delta t = 0.1$ in a 256×256 lattice.*

6.2. Contact process. The contact process is a model of the spreading of infection in a lattice in which a site can be infected via contact with an infected site in its neighborhood [45]. Infection and recovery happen at different rates and there is a critical value of them for which an infection started from a single infected individual will die out in finite time. The contact process with a finite range of infection has a critical dimension $d_c = 4$. At higher dimensions the critical contact process converges to the sBm, but not below d_c. At lower dimensions, it is not known what the scaling limits should be.

However, long-range interaction with suitable scalings shows that the contact process converges to the sBm for $d \geq 2$; see [11]. In one dimension, Mueller and Tribe [35, 36] showed that the rescaled density of particles for the long-range contact process weakly converges to the solution of the SPDE

$$(6.4) \qquad du(x,t) = \left[\Delta u(x,t) + \theta u(x,t) - u(x,t)^2\right] dt + \sqrt{u}\, dW(x,t),$$

where $W(x,t)$ denotes a space-time Wiener process. Moreover, they showed that the above equation undergoes a phase transition at a critical value of θ_c for which

$$(6.5) \qquad \mathcal{P}(u(x,t) \text{ survives}) \begin{cases} = 0 & \text{if } \theta < \theta_c, \\ > 0 & \text{if } \theta > \theta_c. \end{cases}$$

The nontrivial behavior of the solution of (6.4) is believed to represent the well-known universality class for contact processes (also named the directed percolation universality class [23, 34]).

As before, numerical simulations of (6.4) can be now addressed using the splitting scheme and the efficient random number generators for the conditional probability [34]. In particular, we discretize the spatial operators in a lattice $\mathbb{Z}$ (as in (6.2)) and split the dynamics as follows:
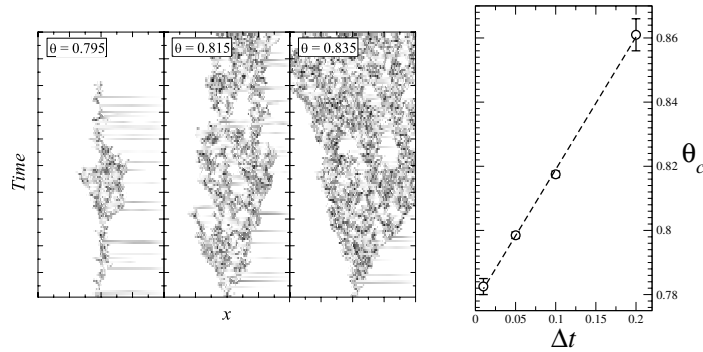
FIG. 6.3. *(Left) Strong path approximation of* (6.4) *for* $\Delta x = 1$ *and* $L = 2^{14}$ *and different values of* θ *below and above the phase transition. (Right) Critical value of* θ_c *as defined in* (6.5) *as a function of* Δt. *The straight line is a linear fit to the data. Parameters are* $\Delta x = 1$, $L = 2^{14}$.

$$(6.6) \qquad du_i^{(1)} = \sqrt{u_i^{(1)}}\, dW(t), \quad du_i^{(2)} = [\Delta_i u_i^{(2)} + \theta u_i^{(2)} - (u_i^{(2)})^2]\, dt,$$

where the last equation is numerically integrated using Euler approximations with sufficiently small step sizes. Results for strong approximations of $u_i(t)$ are shown in Figure 6.3, where we can see a typical realization for the subcritical (infection dies out), critical, and supercritical (infection spreads) for different values of θ.

We can calculate the critical value of θ_c in one dimension using our algorithm. To this end, we identify the critical point θ_c using (6.5) and finite scaling techniques of statistical mechanics. In particular, we found that $\theta_c = 0.777 \pm 0.001$ for $\Delta x = 1$, and the convergence to this value is of order one.

7. Conclusion. The general idea of this paper is to propose a splitting of SDE (1.1) into two new SDEs for which one can keep nonnegativity during integration of both subsystems. This is achieved by either solving one subsystem exactly in the pathwise sense or using its transition probabilities, and solving the other (here nonrandom) subsystem by nonnegativity preserving numerical methods. In this way one is able to preserve nonnegativity and a maximum of convergence order 1.0 in both weak and strong sense. For the efficiency of our splitting algorithm, it is crucial to find a splitting into appropriate subsystems. For this purpose, one also tries to incorporate more complicated boundary conditions of the original SDE (1.1) into an explicitly solvable subsystem such that a fairly easier numerical integration of the remaining subsystem remains to be implemented. For example, for SDEs

$$dX(t) = [\alpha(X(t), t) + \lambda X(t)]\, dt + \sigma X(t)\, dW(t),$$

one makes use of the splitting into

$$dX_1(t) = \lambda X_1(t)\, dt + \sigma X_1(t)\, dW(t), \quad dX_2(t) = \alpha(X_2(t), t)\, dt,$$

where the explicit solution of the first component X_1 is given by

$$X_1(t) = X_1(0) \exp\left(\left(\lambda - \frac{1}{2}\sigma^2\right) t + \sigma W(t)\right),$$

which possesses the monotone property of leaving the positive axes $[0, +\infty)$ invariant by this type of random mapping (almost surely). This idea can be easily extended to

nonlinear systems of SDEs with its splitting into linear and nonlinear subsystems in several dimensions. Another type of splitting is found for nonlinear systems

(7.1) $$dX(t) = f(X(t), t) \, dt + \sigma(X(t), t) \, dW(t)$$

with continuously differentiable coefficients σ as follows. Rewrite this equation as

$$dX(t) = \left[f(X(t), t) - \frac{1}{2}\sigma(X(t), t)\frac{\partial\sigma(X(t), t)}{\partial x} + \frac{1}{2}\sigma(X(t), t)\frac{\partial\sigma(X(t), t)}{\partial x} \right] dt$$
$$+ \sigma(X(t), t) \, dW(t)$$

and set

$$\alpha(x, t) = f(x, t) - \frac{1}{2}\sigma(x, t)\frac{\partial\sigma(x, t)}{\partial x}, \quad \beta(x, t) = \frac{1}{2}\sigma(x, t)\frac{\partial\sigma(x, t)}{\partial x}.$$

Then the splitting-step algorithm is applied to system (X_1, X_2) satisfying (2.2) and (2.3) with coefficients α and β as defined above. This works at least efficiently if $\sigma(x, t) = \sigma(x)$ does not depend on t and the invertible integral $H(z) = \int^z [b(z)]^{-1} \, dz$ exists on the domain of definition of the original equation (7.1) for X. In this case one finds $X_1(t) = H^{-1}(W(t) + H(X_1(0)))$.

Once an appropriate splitting is found then it is relatively easy to implement the related numerical algorithm. The proposed splitting-step method efficiently works since its implementation essentially relies on the well-known variation-of-parameters formula for perturbed dynamical systems which extends to SDEs. Recall that, by this formula, if the equation

$$dX(t) = \beta(X(t), t) \, dt + \sigma(X(t), t) \, dW(t)$$

has known fundamental solution $\Phi = \Phi(t, X_0)$ then the exact solution of the original equation (2.1) possesses the pathwise representation

$$X(t + \Delta t) = \Phi(t + \Delta t, X(t)) + \Phi(t + \Delta t, X(t)) \int_t^{t+\Delta t} [\Phi(s, X(t))]^{-1}\alpha(X(s), s) \, ds$$
$$\approx \Phi(t + \Delta t, X(t)) + \alpha(X(t), t)\Delta t$$

on each subinterval $[t, t + \Delta t] \subset [0, T]$. Thus, the motivation of our splitting-step technique is apparent by finding Φ and numerical integration of $\int \alpha(X(s), s) \, ds$.

Final remark on applicability of our splitting algorithm. The applicability of our splitting algorithm heavily relies on the knowledge on the exact solution of SDEs. An extensive list of analytically known solutions is found in textbooks such as [27]. Of course, in one dimension one knows more about explicitly solvable SDEs. However, our technique is also applicable to multidimensional problems. For example, when noise terms are linear, decoupled, commutative, or diagonal, one can apply it successfully, too. In particular, the knowledge of explicitly solvable linear multidimensional stochastic subsystems from appropriately split systems can be exploited (see also Appendix C). So we are not exclusively restricted to one-dimensional problems (although we must admit that the range of highly efficient applicability may shrink with the increase of dimensions). A more detailed discussion on multidimensional extensions of splitting techniques is left to research in the future. We have deliberately chosen some well-known examples from the literature such that the interested

reader may easily compare the performance of his preferred numerical technique to our semianalytic numerical splitting technique.

Appendix A. Noncentral chi-square distribution random number generation. The splitting-step method proposed in this paper relies on the exact numerical sampling of transition probability density for some processes. In particular, efficient generation of random numbers $\chi_d'^2(\lambda)$ with a noncentral chi-square distribution with d degrees of freedom whose probability density function is found by

$$(A.1) \quad \mathcal{P}[\chi_d'^2(\lambda) = x] = p(x; d, \lambda) = \frac{e^{-(\lambda+x)/2}}{2} \left(\frac{x}{\lambda}\right)^{(d-2)/4} I_{(\nu-2)/2}(\sqrt{\lambda x}), \quad x > 0,$$

in [24]. This distribution is properly defined for any positive d and was extended to the case $d = 0$ by Siegel [44]. Here we shall extend it to the case $d = -2, -4, \ldots$ and show how to sample this distribution.

To this end, we use the fact that the distribution (A.1) can be expressed also as a mixture of central χ^2 variables with Poisson weights

$$(A.2) \qquad p(x; d, \lambda) = \sum_{j=0}^{\infty} \frac{(\lambda/2)^j e^{-\lambda/2}}{j!} p_0(x; d + 2j), \quad d > 0,$$

where $p_0(x; d)$ is the distribution of a chi-square random variable χ_d^2 with d degrees of freedom. This expression suggests a simple and efficient procedure to obtain $\chi_d'^2(\lambda)$ random variables:

1. Choose K from a Poisson distribution with mean $\lambda/2$ so that $\mathcal{P}[K = k] = e^{-k/2}(\lambda/2)^k/k!$ $(k = 0, 1, \ldots)$.
2. Then take $\chi_d'^2(\lambda) = \chi_{d+2K}^2$, which can be done using the any standard random number generator of the χ_d^2 distribution.

In the $d = 0$ case, the $\chi_d'^2(\lambda)$ distribution has a discrete component at zero with mass $e^{\lambda/2}$ (which represents the probability to get absorbed at zero in our stochastic processes); see [44]. We have

$$(A.3) \qquad p(x; 0, \lambda) = \sum_{j=1}^{\infty} \frac{(\lambda/2)^j e^{-\lambda/2}}{j!} p_0(x; 2j) + e^{-\lambda/2}\delta(x), \quad d = 0.$$

The procedure above can be modified to account for this discrete component by taking the convention that the central χ_d^2 distribution is identically zero when $d = 0$. This convention can be extended to even negative dimensions to get

$$(A.4) \qquad p(x; d, \lambda) = \sum_{j=|d|/2+1}^{\infty} \frac{(\lambda/2)^j e^{-\lambda/2}}{j!} p_0(x; d + 2j) + \delta(x) \sum_{j=0}^{|d|/2} \frac{(\lambda/2)^j e^{-\lambda/2}}{j!}$$

for $d = 0, -2, -4, \ldots$.

Summarizing, if K is a Poisson random number with mean $\lambda/2$ we have

$$(A.5) \qquad\qquad\qquad \chi_d'^2(\lambda) = \chi_{d+2K}^2, \qquad d > 0,$$

and

$$(A.6) \qquad \chi_d'^2(\lambda) = \begin{cases} 0 & \text{if } d + 2K \leq 0, \\ \chi_{d+2K}^2 & \text{if } d + 2K > 0, \end{cases} \qquad d = 0, -2, -4, \ldots.$$

This sampling of the probability distribution function is exact and should be used especially when λ is small. However, when λ is large, the $\chi_d'^2(\lambda)$ distribution asymptotically converges to the Gaussian distribution and other approximations (like the ones in [24]) might be considered to improve the speed of our algorithm.

Appendix B. Numerical generation of strong path solutions for some processes. The success of the splitting-step method requires the exact numerical integration of step 1 which can be problematic in some situations. That is why we have applied in previous numerical examples such equations which allow us to represent the solution from step 1 in terms of pure functions of the Wiener process and initial values such as $X(t) = F(X(0), W(t))$ or simple deterministic integrals as seen with the example of Bessel-type diffusions $X(t) = (\sqrt{X(0)} + W(t))^2$ or the geometric Brownian motion $X(t) = X(0)\exp((\alpha - \sigma^2/2)t + \sigma W(t))$. Also, for the Ornstein–Uhlenbeck processes or logistic equations, one may use the well-known integration-by-parts formula and / or the information on the exact distribution of involved stochastic integrals with deterministic differentials which can be pathwisely treated by deterministic quadrature methods. As another alternative, one could exploit the Doss representation (see [9]) to develop a semianalytic approach or an ODE-PDE approach to decompose the original problem into a random ODE and a deterministic PDE in order to figure out which numerical implementation is more efficient in conjunction with our splitting technique. However, in general one produces additional discretization errors which might influence the accuracy of the computations using the splitting algorithm as well. Then it is a must to consider its stability properties too. Such a fairly complex and very problem-dependent work is left to the future.

Appendix C. A general theorem on L^2-convergence based on the VOP. To exploit the specific knowledge on solvability of bilinear stochastic systems, once may also make use of the well-known variation-of-constants formula (VOP) (this formula is also sometimes called the variation-of-parameters formula). This possibility is justified through this section. For this purpose, suppose that the original equation is

$$(C.1) \quad dX(t) = [\alpha(X(t), t) + \beta(t)X(t)]\,dt + \sigma_2(X(t), t)\,dW_2(t) + \sigma_1(t)X(t)\,dW_1(t),$$

where W_1 and W_2 are independent Wiener processes. Consider the splitting

$$(C.2) \qquad\qquad dX_1(t) = \beta(t)X_1(t)\,dt + \sigma_1(t)X_1(t)\,dW_1(t),$$
$$(C.3) \qquad\qquad dX_2(t) = \alpha(X_2(t), t)\,dt + \sigma_2(X_2(t), t)\,dW_2(t)$$

with Borel-measurable real-valued matrices $\beta(t), \sigma_1(t) \in \mathbb{R}^{d\times d}$. Let $C_{locLip}^0(S)$ denote the vector space of local Lipschitz continuous functions on the open set S.

THEOREM C.1. *Assume that the coefficient functions $\alpha, \sigma_2 \in C_{locLip}^0(\mathbb{D} \times [0, T])$ and $\beta, \sigma_1 \in \mathbb{R}^{d\times d}$ are such that the continuous unique strong solution X of (C.1) exists on the closed set $\bar{\mathbb{D}}$,*

$$\sup_{0\leq t\leq T} \mathbb{E}\left[|X(t)|^2\right] + \sup_{0\leq t<T}\sup_{t\leq s\leq T} \mathbb{E}\left[|\Phi(s, X(t))|^2\right] < +\infty,$$

$$\sup_{0\leq t\leq T} \mathbb{E}\left[\int_t^T |[\Phi(s, X(t))]^{-1}\alpha(X(s), s)|^2\,ds + \int_t^T |[\Phi(s, X(t))]^{-1}\sigma_2(X(s), s)|^2\,ds\right] < +\infty$$

for a fixed, finite, nonrandom terminal time $T > 0$ and the stochastic flow Φ generated by (C.2) is mean square Hölder-continuous with exponent $r_H \geq 0.5$. Furthermore,

suppose that step 1 *of the splitting algorithm is exactly integrable and step* 2 *can be carried out with local mean accuracy with rate* $r_1 \geq 1.0$, *local mean square accuracy with rate* $r_2 \geq 0.5$, *and* $\min(r_1, r_H + 1.0) \geq \min(r_2, r_H + 1.0) + 0.5$.

Then, in the worst case, the error of the splitting-step algorithm with steps 1 *and* 2 *has*

$$r_g \geq \min(1.0, \min(r_2, r_H + 1.0) - 0.5)$$

as its (global) rate of L^2-*convergence on the interval* $[0, T]$.

Remark. The VOP is needed for the proof. This formula for the perturbation of Itô-interpreted fundamental systems

$$\text{(C.4)} \qquad dX(t) = A(t)X(t)\,dt + \sum_{j=1}^{m} B_j(t)X(t)\,dW_j(t)$$

with real-valued matrices $A(t)$ and $B(t) \in \mathbb{R}^{d \times d}$ by

$$\text{(C.5)} \qquad dX(t) = [A(t)X(t) + f(t)]\,dt + \sum_{j=1}^{m}[B_j(t)X(t) + g_j(t)]\,dW_j(t)$$

with vector-valued random functions f and g_j can be found as Theorem 3.1 from Mao [30, pp. 96–97]. It says that systems (C.5) have the representation

$$X(s) = \Phi(s)\left(X(t) + \int_t^s [\Phi(u)]^{-1}\left[f(u) - \sum_{j=1}^{m} B_j(u)g_j(u)\right]du\right.$$

$$\text{(C.6)} \qquad\qquad\qquad \left. + \sum_{j=1}^{m}\int_t^s [\Phi(u)]^{-1}g_j(u)\,dW_j(u)\right)$$

in terms of the fundamental solution Φ related to linear system (C.4), where $s \geq t$. Thus, it heavily relies on the specific knowledge of properties of the flow Φ of underlying linear fundamental systems (C.4). Note that autonomous systems (C.4) with $m = 1$, constant matrices A, B, and commutativity condition $[A, B] = AB - BA = 0$ possess the explicit representation in terms of matrix exponentials (for $s \geq t$)

$$\Phi(s, X(t)) = \exp\left(\left(A - \frac{1}{2}B^2\right)(s - t) + B(W(s) - W(t))\right)X(t).$$

Proof. Suppose that (C.2) has known fundamental solution $\Phi = \Phi(t, X_0)$ with a.s. Hölder exponent r_H. Then, following the VOP (C.6) (see the above remark), the exact solution of the original equation (C.1) possesses the pathwise representation

$$X(t + \Delta t) = \begin{cases} \Phi(t + \Delta t, X(t)) \\[2mm] + \Phi(t + \Delta t, X(t))\displaystyle\int_t^{t+\Delta t}[\Phi(s, X(t))]^{-1}\alpha(X(s), s)\,ds \\[2mm] + \Phi(t + \Delta t, X(t))\displaystyle\int_t^{t+\Delta t}[\Phi(s, X(t))]^{-1}\sigma_2(X(s), s)\,dW_2(s) \end{cases}$$

on each subinterval $[t, t + \Delta t] \subset [0, T]$. Note that formula (C.6) is applied with

$$A(s) = \beta(s), \quad B_1(s) = \sigma_1(s), \quad B_2(s) = 0,$$
$$f(s) = \alpha(X(s), s), \quad g_1(s) = 0, \quad g_2(s) = \sigma(X(s), s).$$

Now, let $Y(t)$ denote the value of right-continuous numerical approximation of splitting step algorithm (which we always can construct using step functions in a standard way). The main idea is to apply the fairly general L^2-convergence theory known from [31, 41, 42, 43]. For this purpose, we need to study the local conditional accuracy of our algorithm. Locally, we may suppose that $X(t) = Y(t) = x$ is deterministic ($\mathcal{F}_t$-adapted). First, consider the local conditional mean accuracy. We find that

$$
\left| \mathbb{E}\left[X(t + \Delta t) - Y(t + \Delta t) \middle| \mathcal{F}_t \right] \right|
$$

$$
= \left| \mathbb{E}\left[\Phi(t + \Delta t, x) \int_t^{t+\Delta t} [\Phi(s,x)]^{-1} \alpha(X(s), s)\, ds \right. \right.
$$

$$
\left. \left. + \Phi(t + \Delta t, x) \int_t^{t+\Delta t} [\Phi(s,x)]^{-1} \sigma_2(X(s), s)\, dW_2(s) - (Y(t + \Delta t) - x) \middle| \mathcal{F}_t \right] \right|
$$

$$
\leq \left| \mathbb{E}\left[\int_t^{t+\Delta t} \left(\Phi(t + \Delta t, x) - \Phi(s, x) \right) [\Phi(s,x)]^{-1} \alpha(X(s), s)\, ds \middle| \mathcal{F}_t \right] \right|
$$

$$
+ \left| \mathbb{E}\left[\int_t^{t+\Delta t} \left(\Phi(t + \Delta t, x) - \Phi(s, x) \right) [\Phi(s,x)]^{-1} \sigma_2(X(s), s)\, dW_2(s) \middle| \mathcal{F}_t \right] \right|
$$

$$
+ \left| \mathbb{E}\left[\int_t^{t+\Delta t} \alpha(X(s), s)\, ds + \int_t^{t+\Delta t} \sigma_2(X(s), s)\, dW_2(s) - (Y(t + \Delta t) - x) \middle| \mathcal{F}_t \right] \right|
$$

$$
\leq K_1 [\Delta t]^{\min(r_1, (2r_H+1)/2+0.5)},
$$

where K_1 is a real constant; hence the local conditional mean accuracy rate

$$
\min(r_1, (2r_H + 1)/2 + 0.5) = \min(r_1, r_H + 1.0)
$$

of the splitting algorithm can be verified. Second, consider the local conditional mean square accuracy of the splitting algorithm:

$$
\left(\mathbb{E}\left[|X(t + \Delta t) - Y(t + \Delta t)|^2 \middle| \mathcal{F}_t \right] \right)^{1/2}
$$

$$
= \left(\mathbb{E}\left[\left| \Phi(t + \Delta t, x) \int_t^{t+\Delta t} [\Phi(s,x)]^{-1} \alpha(X(s), s)\, ds \right. \right. \right.
$$

$$
\left. \left. \left. + \Phi(t + \Delta t, x) \int_t^{t+\Delta t} [\Phi(s,x)]^{-1} \sigma_2(X(s), s)\, dW_2(s) - (Y(t + \Delta t) - x) \right|^2 \middle| \mathcal{F}_t \right] \right)^{1/2}
$$

$$
\leq \left(\mathbb{E}\left[\left| \int_t^{t+\Delta t} \left(\Phi(t + \Delta t, x) - \Phi(s, x) \right) [\Phi(s,x)]^{-1} \alpha(X(s), s)\, ds \right|^2 \middle| \mathcal{F}_t \right] \right)^{1/2}
$$

$$
+ \left(\mathbb{E}\left[\left| \int_t^{t+\Delta t} \left(\Phi(t + \Delta t, x) - \Phi(s, x) \right) [\Phi(s,x)]^{-1} \sigma_2(X(s), s)\, dW_2(s) \right|^2 \middle| \mathcal{F}_t \right] \right)^{1/2}
$$

$$
+ \left(\mathbb{E}\left[\left| \int_t^{t+\Delta t} \alpha(X(s), s)\, ds + \int_t^{t+\Delta t} \sigma_2(X(s), s)\, dW_2(s) - (Y(t + \Delta t) - x) \right|^2 \middle| \mathcal{F}_t \right] \right)^{1/2}
$$

$$
\leq K_2 [\Delta t]^{\min(r_2, (2r_H+1)/2+0.5)},
$$

where K_2 is a real constant; hence the local conditional mean square accuracy rate

$$\min(r_2, (2r_H + 1)/2 + 0.5) = \min(r_2, r_H + 1.0)$$

of the splitting algorithm can be derived. Now, apply the general convergence theory from [31, 41, 42, 43] to conclude the worst case estimate of global mean square convergence rate r_g as stated in Theorem C.1 along nonrandom partitions of $[0, T]$.   □

Example. Consider the Itô-interpreted example

(C.7) $$dX(t) = (1 + X(t))\, dt + \sqrt{2}X(t)\, dW_1(t) + 2\sqrt{X(t)}\, dW_2(t).$$

Clearly, SDE (C.7) is of the form (C.1) with $\alpha(X, t) = 1$, $\beta(t) = 1$, $\sigma_2(X, t) = 2\sqrt{X(t)}$, and $\sigma_1(t) = \sqrt{2}$. Moreover, this example satisfies the assumptions of Theorem C.1 with $r_H = 0.5$. To see this fact, use the splitting into the subsystems

(C.8) $$dX_1(t) = X_1(t)\, dt + \sqrt{2}X_1(t)\, dW_1(t),$$

(C.9) $$dX_2(t) = dt + 2\sqrt{X_2(t)}\, dW_2(t).$$

The stochastic flows Φ_i related to linear (C.8) and nonlinear subsystems (C.9) are

$$\Phi_1(s, x) = \exp(\sqrt{2}W_1(s))x, \quad \Phi_2(s, x) = (\sqrt{x} + W_2(s))^2$$

as direct applications of Itô's formula. Besides, both flows have uniformly bounded moments of all orders for nonrandom initial data and they are mean square Hölder-continuous with exponent $r_H = 0.5$. For example, for the second subsystem (C.9), we have $\Phi_2(t, X(0)) - \Phi_2(s, X(0)) = 2\sqrt{X(0)}(W_2(t) - W_2(s))$ and

$$\mathbb{E}\, |\Phi_2(t, X(0)) - \Phi_2(s, X(0))|^2 = 2\,\mathbb{E}\,[X(0)]\,\mathbb{E}\,|W_2(t) - W_2(s)|^2 = 2\,\mathbb{E}\,[X(0)]\,|t - s|$$

provided that $X(0) \geq 0$ (a.s.) is independent of the processes W_2. Therefore, the related splitting-step algorithm can be applied and achieve a global L^2-convergence order $r_g = 1.0$ since the splitting-step integration has trivially at least local accuracy rates $r_1 = 2.0$ and $r_2 = 1.0$ thanks to the exact knowledge on the analytic expression of both subflows and the formula for r_g given by Theorem C.1. Moreover, the positivity-preserving character of such a splitting technique is obvious from the explicit formulas of subflows Φ_i. Similarly, we can proceed for other equations with $\sqrt{(.)}$- or other Hölder-continuous terms with Hölder exponent ≥ 0.5.

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