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EXPONENTIAL TIMESTEPPING WITH BOUNDARY TEST FOR STOCHASTIC DIFFERENTIAL EQUATIONS*

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Abstract. We present new numerical methods for scalar stochastic differential equations. Successive time increments are independent random variables with an exponential distribution. We perform numerical experiments using a double-well potential. Exponential timestepping algorithms are efficient for escape-time problems because a simple boundary test can be performed at the end of each step.

Key words. stochastic calculus, numerical methods, a posteriori error estimates, diffusion with boundaries

AMS subject classifications. 60-08, 65C30

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1. Introduction. Approximate numerical solutions of stochastic differential equations are produced by recursively updating an approximating process at discrete times [1, 2, 3, 4, 5, 6]. The case where the interval between successive times is a random variable with an exponential distribution has been analyzed and applied to the simplest stochastic process, the Wiener process; an exact update is possible without generating Gaussian random variables and boundaries can be efficiently taken into account at each timestep [7]. Here we consider scalar processes satisfying stochastic differential equations of the following form:

$$\mathrm{d}\mathbf{X}_t = f(\mathbf{X}_t)\mathrm{d}t + \sigma(\mathbf{X}_t)\,\mathrm{d}\mathbf{W}_t. \tag{1.1}$$

The process $\mathbf{X}$ has continuous paths and takes values on the real line. In the simplest algorithm, the stochastic Euler algorithm, an update is produced as follows:

$$\mathbf{X}_{t+\Delta t} - \mathbf{X}_t = f(\mathbf{X}_t)\Delta t + \sigma(\mathbf{X}_t)(\Delta t)^{\frac{1}{2}}\mathbf{n}, \tag{1.2}$$

where $\mathbf{n}$ is a Gaussian random variable with mean zero and variance 1. The duration of the timestep, Δt, is predetermined. Under exponential timestepping, successive time increments are independent realizations of an exponentially distributed random variable $\boldsymbol{\delta t}$:

$$\mathcal{P}[\boldsymbol{\delta t} > t] = \exp(-\lambda t). \tag{1.3}$$

We shall describe how to produce an update under this exponential timestepping.

One of the most difficult tasks for existing numerical methods is the measurement of exit times, where the quantity of interest is the first time that a process attains a given value or exits a region. Even if updates of the process are generated with good accuracy, large errors can result from the possibility that the boundary is reached

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during a timestep although the process is within the boundary at both the beginning and the end of the timestep [7, 8, 9, 10, 11]. At the end of each exponential timestep, we perform a simple a posteriori test for this possibility, based on the value of the process at the start and end of the timestep. The required conditional probabilities have a simple form under exponential timestepping, which can be thought of as corresponding to a fixed probability per unit time of the timestep coming to an end. In particular, the distribution of the value taken by the process at the end of the timestep, given that the point b is attained during the timestep, is the same as if the timestep had started at b.

An exponential timestep with boundary test is performed as follows. We first update the process. Then we test for the possibility of a boundary having been reached in the time interval. In section 2 we calculate the quantities needed in order to carry out this procedure: the density of the random variable $\mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t$ and the conditional probability of having attained a given value during the timestep. Both quantities can be written in a convenient form, in terms of solutions of a linear homogeneous differential equation. In section 3 we analyze several types of process satisfying (1.1) in more detail. In section 4 we implement two algorithms for exponential timestepping and perform numerical experiments to compare their properties with those of fixed-step algorithms.

2. Basic results. We consider an exponential timestep for a process satisfying (1.1). Because all quantities are independent of the starting time, we take a step started at $t = 0$. We shall be interested in the density of values of $\mathbf{X}_{\boldsymbol{\delta t}}$ and the probability that the process attains a value, denoted b, before $\boldsymbol{\delta t}$. Let

$$\mathbf{H}_b^{\mathbf{X}}(x) = \inf\{t > 0 : \mathbf{X}_t = b \,|\mathbf{X}_0 = x\}. \tag{2.1}$$

Then [12, 13, 14, 15]

1. if $b > x$,

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t}] = \phi^{\uparrow}(x)/\phi^{\uparrow}(b); \tag{2.2}$$

2. if $b < x$,

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t}] = \phi^{\downarrow}(x)/\phi^{\downarrow}(b). \tag{2.3}$$

The notation $\phi^{\uparrow}(x)$ and $\phi^{\downarrow}(x)$ is used to distinguish the increasing and decreasing functions of x. Both functions satisfy the following differential equation [13, 14, 15, 16]:

$$\frac{1}{2}\sigma(x)^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi(x) + f(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) = \lambda\phi(x). \tag{2.4}$$

The pair of independent positive solutions of (2.4), $\phi^{\uparrow}(x)$ and $\phi^{\downarrow}(x)$, are defined up to a multiplicative constant by [12, 14]:

$$\lim_{x\to-\infty} \phi^{\uparrow}(x) = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x) > 0 \tag{2.5}$$

and

$$\lim_{x\to\infty} \phi^{\downarrow}(x) = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}x}\phi^{\downarrow}(x) < 0. \tag{2.6}$$

Note that the duration of the timestep enters (2.4) through the parameter λ; the only derivatives in (2.4) are with respect to x.

It is useful to think of the exponential distribution of $\boldsymbol{\delta t}$ as corresponding to a fixed probability per unit time of the timestep coming to an end. One consequence of this equivalence is that the distribution of the value taken by the process at the end of the timestep, given that the point b is attained during the timestep, is the same as if the timestep had started at b:

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t},\ \mathbf{X}_{\boldsymbol{\delta t}} < y] = \mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t}]\mathcal{P}[\mathbf{X}_{\boldsymbol{\delta t}} < y | \mathbf{X}_0 = b]. \tag{2.7}$$

We write the density of $\mathbf{X}_{\boldsymbol{\delta t}}$ as follows:

$$R(x, y) = \frac{\mathrm{d}}{\mathrm{d}y}\mathcal{P}[\mathbf{X}_{\boldsymbol{\delta t}} < y | \mathbf{X}_0 = x]. \tag{2.8}$$

Given $\mathbf{X}_t = x$, the probability that $\mathbf{X}_{t+\boldsymbol{\delta t}}$ falls in an interval (l, r) is given as

$$\mathcal{P}[\mathbf{X}_{\boldsymbol{\delta t}} \in (l, r) | \mathbf{X}_0 = x] = \int_l^r R(x, y)\mathrm{d}y. \tag{2.9}$$

The corresponding probability, with the additional condition that b is attained during the interval, is obtained from (2.8) and (2.7):

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t},\ \mathbf{X}_{\boldsymbol{\delta t}} \in (l, r)] = \mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t}] \int_l^r R(b, y)\mathrm{d}y. \tag{2.10}$$

To obtain the probability of having reached b, given that the timestep starts at x and finishes at y, we divide (2.10) by (2.9):

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t} | \mathbf{X}_{\boldsymbol{\delta t}} = y] = \mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t}] \frac{R(b, y)}{R(x, y)}. \tag{2.11}$$

The density $R(x, y)$ can itself be expressed in terms of the functions $\phi^{\uparrow}(x)$ and $\phi^{\downarrow}(x)$ [13, 14, 15]:

$$R(x, y) = N\, m(y)\phi^{\uparrow}(x \wedge y)\phi^{\downarrow}(x \vee y), \tag{2.12}$$

where $x \wedge y = \min(x, y)$ and $x \vee y = \max(x, y)$,

$$m(x) = 2\sigma^{-2}(x) \exp\left(2 \int_0^x \frac{f(y)}{\sigma^2(y)}\, \mathrm{d}y\right), \tag{2.13}$$

and N is a normalization constant (see Appendix A).

Suppose $x < b$ and $y < b$. Then, using (2.2) and (2.12), the conditional probability (2.11) can be written

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t} | \mathbf{X}_{\boldsymbol{\delta t}} = y] = \frac{\phi^{\uparrow}(x \vee y)}{\phi^{\uparrow}(b)} \frac{\phi^{\downarrow}(b)}{\phi^{\downarrow}(x \vee y)}\ . \tag{2.14}$$

Notice that, given $\mathbf{X}_t = x$ and $\mathbf{X}_{t+\boldsymbol{\delta t}} = y$, the probability of having reached b during the timestep is dependent only on b and on the maximum of x and y (see Figure 2.1). Similarly, if $x > b$ and $y > b$,

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t} | \mathbf{X}_{\boldsymbol{\delta t}} = y] = \frac{\phi^{\downarrow}(x \wedge y)}{\phi^{\downarrow}(b)} \frac{\phi^{\uparrow}(b)}{\phi^{\uparrow}(x \wedge y)}, \tag{2.15}$$

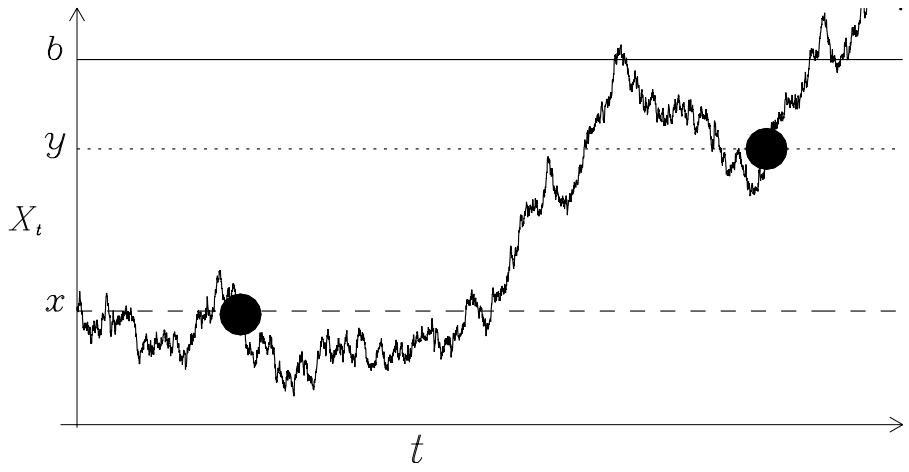

FIG. 2.1. *The beginning and the end of the timestep are marked with black circles. The value of the process at the beginning of the timestep is x; the value at the end is y. Even if both x and y are known to high accuracy, and both are on the same side of b, the level b can be reached for an intermediate time, as is the case in the path shown. When the length of the timestep is an exponentially distributed random variable, the probability of such an event is a function of b and of the closer of x and y to b.*

a function only of b and the minimum of x and y.

For the simplest stochastic process, the Wiener process with $f(x) = 0$ and $\sigma(x) = 1$, the increasing and decreasing solutions of (2.4) are $\phi^{\uparrow}(x) = \exp(\sqrt{2\lambda}x)$ and $\phi^{\downarrow}(x) = \exp(-\sqrt{2\lambda}x)$. The conditional probabilities (2.14) and (2.15) are $\mathcal{P}[\mathbf{H}_b^{\mathbf{W}}(x) < \boldsymbol{\delta t}|\mathbf{X}_{\boldsymbol{\delta t}} = y] = \exp\left(-2(b - (x \vee y))\right)$ if $x < b$ and $y < b$, or $\mathcal{P}[\mathbf{H}_b^{\mathbf{W}}(x) < \boldsymbol{\delta t}|\mathbf{X}_{\boldsymbol{\delta t}} = y] = \exp\left(-2((x \wedge y) - b)\right)$ if $x > b$ and $y < b$. Another case where a simple exact formula can be found is considered in section 3. In general such formulae are not available, but the property that the conditional hitting probability depends only on the closer of the starting point and the ending point to b is maintained, as can be seen from the following argument. Consider the case $x < b$ and $y < b$. If $y < x$, the portion of the path between time t and time $t + \boldsymbol{\delta t}$ can be divided up into a series of excursions from the level x, plus the final portion from x until the end of the timestep at $\mathbf{X}_{t+\boldsymbol{\delta t}} = y$. Each of the excursions is independent, and independent of what happens in the final portion of the path. In particular, the probability of reaching the level b during one of the excursions depends on x but is independent of y. In the other case, when $y \geq x$, we can divide the path up into the first portion from time t until the first time that the value y is reached, followed by a series of excursions from y. The probability of reaching b during one of these excursions is independent of x. Similar arguments hold if $x > b$ and $y > b$. By contrast, when the time taken to go from x to y is fixed, the excursions are constrained to have a total time equal to a given number and are not independent. For this reason, conditional hitting probabilities have less convenient (or nonexistent) analytical forms when the duration of the timestep is a known quantity.

3. Exponential timestepping with boundaries. In this section we analyze the solutions of the differential equation (2.4) under various hypotheses for $f(x)$ and $\sigma(x)$. In all cases we require that $\sigma^2(x) > 0$ and that $f(x)$ is such that solutions cannot escape to infinity in a finite time. Section 3.1 deals with the simple case where

both $f(x)$ and $\sigma(x)$ are constants; exact analytical expressions can be found for the density of increments and for the conditional probability of having reached a boundary during a timestep. In section 3.2, the case of "additive noise" is considered: $f(x)$ is a nonlinear function but $\sigma(x) = \epsilon$, a constant. We expand the solutions $\phi^{\uparrow}(x)$ and $\phi^{\downarrow}(x)$ in powers of ν^{-1} where $\nu = (2\lambda/\epsilon^2)^{\frac{1}{2}}$. In section 3.3 we tackle the case where both $f(x)$ and $\sigma(x)$ are nonconstant, via a WKB-type expansion.

3.1. Brownian motion with constant drift. Exact calculations can be performed when $f(x)$ and $\sigma(x)$ are constant. To aid readability, we shall use the symbol $\mathbf{Y}_t$ for the constant drift process:

$$\mathbf{Y}_t = \mu t + \epsilon \mathbf{W}_t, \qquad \mathbf{Y}_0 = 0, \tag{3.1}$$

for constant μ and ϵ. A process of this type is usually called Brownian motion with constant drift. The corresponding differential equation (2.4) is linear with constant coefficients and has the following solutions:

$$\phi^{\downarrow}(x) = \exp\left(-(\tilde{\nu} + U)x\right) \quad \text{and} \quad \phi^{\uparrow}(x) = \exp\left((\tilde{\nu} - U)x\right), \tag{3.2}$$

where

$$U = \frac{\mu}{\epsilon^2} \quad \text{and} \quad \tilde{\nu} = \left(\nu^2 + U^2\right)^{\frac{1}{2}}. \tag{3.3}$$

The density of increments of $\mathbf{Y}$ under exponential timestepping, defined in (2.8), can now be obtained from (2.12). In this simple case, however, it is possible to obtain the same result, using the fact that the distance traveled by the process, starting from any x_0, after a fixed time t is a Gaussian random variable with mean μt and variance $\epsilon^2 t$. Integrating over the exponential density of possible values of $\boldsymbol{\delta t}$ yields

$$\begin{aligned} R(x_0, x_0 + x) &= \int_0^{\infty} \lambda \exp(-\lambda t) \left(2\pi\epsilon^2 t\right)^{-\frac{1}{2}} \exp\left(-(x - \mu t)/2\epsilon^2 t\right) \mathrm{d}t \\ &= \frac{\lambda}{\epsilon^2}\, \tilde{\nu}^{-1} \exp\left(-|x|\tilde{\nu} + Ux\right). \end{aligned} \tag{3.4}$$

The density (3.4) is exponential for positive and negative x, with a slower decay when x and U have the same sign. In particular, integrating (3.4) gives

$$\mathcal{P}[\mathbf{Y}_{t+\boldsymbol{\delta t}} > \mathbf{Y}_t] = \frac{1}{2}\left(1 + \frac{U}{\tilde{\nu}}\right). \tag{3.5}$$

Consider an exponential timestep started at $t = 0$. The probability that a boundary, a distance b above the starting point of the step, is reached during an exponential timestep is evaluated using (2.2):

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{Y}}(x) < \boldsymbol{\delta t}] = \exp\left(-(\tilde{\nu} - U)(b - x)\right). \tag{3.6}$$

Suppose $\mathbf{Y}_t = x$ and $\mathbf{Y}_{t+\boldsymbol{\delta t}} = y$ where both $x < b$ and $y < b$. The *conditional* probability that $\mathbf{Y}_s = b$ for some time s in the interval $(0, \boldsymbol{\delta t})$ is

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{Y}}(x) < \boldsymbol{\delta t} | \mathbf{Y}_{\boldsymbol{\delta t}} = y] = \exp\left(-2\tilde{\nu}\left(b - (x \vee y)\right)\right). \tag{3.7}$$

Similarly, if $x > b$ and $y > b$, then

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{Y}}(x) < \boldsymbol{\delta t} | \mathbf{Y}_{\boldsymbol{\delta t}} = y] = \exp\left(-2\tilde{\nu}\left((x \wedge y) - b\right)\right). \tag{3.8}$$

3.2. Additive noise. We now consider the case $\sigma(x) = \epsilon$, where ϵ is constant, but $f(x)$ is a function of x. This case is known as additive noise because the intensity of the noise is independent of the value of the process and can be considered as a random addition to an ordinary differential equation [17]. The differential equation (2.4) satisfied by the function $\phi^{\uparrow}(x)$ reduces to

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi^{\uparrow}(x) + 2\epsilon^{-2} f(x) \frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x) = \nu^2 \phi^{\uparrow}(x), \tag{3.9}$$

where $\nu = \left(2\lambda/\epsilon^2\right)^{\frac{1}{2}}$.

To develop a series solution of (3.9), we define the function $h(x)$ by

$$\phi^{\uparrow}(x) = \exp\left(\nu \int_0^x h(z)\,\mathrm{d}z\right). \tag{3.10}$$

The differential equation satisfied by $h(x)$ is

$$h^2(x) + \nu^{-1}\left(\frac{\mathrm{d}}{\mathrm{d}x}h(x) + 2\epsilon^{-2} f(x)\, h(x)\right) = 1. \tag{3.11}$$

We shall use the parameter ν^{-1} as a small parameter and seek a solution of the following form:

$$h(x) = h_0(x) + \nu^{-1} h_1(x) + \nu^{-2} h_2(x) + \cdots. \tag{3.12}$$

To $\mathcal{O}(1)$, using the condition (2.5), we obtain

$$h_0(x) = 1. \tag{3.13}$$

To $\mathcal{O}(\nu^{-1})$, we find

$$h_1(x) = -\epsilon^{-2} f(x). \tag{3.14}$$

The solution $\phi^{\uparrow}(x)$ can thus be expanded as

$$\phi^{\uparrow}(x) = \exp\left(\nu x + \epsilon^{-2} V(x) + \mathcal{O}(\nu^{-1})\right), \tag{3.15}$$

where the "potential" function $V(x)$ is given by

$$V(x) = -\int_0^x f(z)\,\mathrm{d}z. \tag{3.16}$$

Similarly, using (2.6), we find

$$\phi^{\downarrow}(x) = \exp\left(-\nu x + \epsilon^{-2} V(x) + \mathcal{O}(\nu^{-1})\right). \tag{3.17}$$

The density of the increments of $\mathbf{X}$ is therefore given by

$$R(x,y) = N \exp\left(-\nu|y-x| - \epsilon^{-2}(V(y) - V(x)) + \mathcal{O}(\nu^{-1})\right), \tag{3.18}$$

where

$$N = \frac{\nu}{2}\left(1 + \mathcal{O}(\nu^{-2})\right).$$

The increments are not symmetric about 0 if $f(\mathbf{X}_t) \neq 0$:

$$\mathcal{P}[\mathbf{X}_{t+\boldsymbol{\delta t}} > \mathbf{X}_t] = \frac{1}{2}\left(1 + \nu^{-1}\epsilon^{-2} f(\mathbf{X}_t) + \mathcal{O}(\nu^{-2})\right). \tag{3.19}$$

The *conditional* probability that $\mathbf{X}_s = b$ for some time s in the interval $(t, t+\boldsymbol{\delta t})$ is,

1. if $b > x$ and $b > y$,

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t} | \mathbf{X}_{\boldsymbol{\delta t}} = y] = \exp\left(-2\nu(b - (x \vee y)) + \mathcal{O}(\nu^{-1})\right), \tag{3.20}$$

2. if $b < x$ and $b < y$,

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \boldsymbol{\delta t} | \mathbf{X}_{\boldsymbol{\delta t}} = y] = \exp\left(-2\nu((x \wedge y) - b) + \mathcal{O}(\nu^{-1})\right). \tag{3.21}$$

3.3. Multiplicative noise. When both $f(x)$ and $\sigma(x)$ are nonconstant, the differential equation (2.4) can be put in a form amenable to WKB-type analysis [18, 19]:

$$\lambda^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi^{\uparrow}(x) + \lambda^{-1}2\sigma^{-2}(x)f(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x) = 2\sigma^{-2}(x)\phi^{\uparrow}(x). \tag{3.22}$$

When $\sigma(x)$ is bounded away from 0, we can carry out an expansion of the solution in the standard form

$$\phi^{\uparrow}(x) = \exp\left(\sum_{n=0}^{\infty}\delta^{n-1}S_n^{\uparrow}(x)\right), \qquad \phi^{\downarrow}(x) = \exp\left(\sum_{n=0}^{\infty}\delta^{n-1}S_n^{\downarrow}(x)\right). \tag{3.23}$$

The appropriate small parameter is $\delta = (2\lambda)^{-\frac{1}{2}}$. Note that both terms on the left-hand side in (3.22) are multiplied by λ^{-1}.

The first two functions in the expansion (3.23) satisfy

$$\frac{\mathrm{d}}{\mathrm{d}x}S_0^{\uparrow}(x) = \sigma^{-1}(x), \qquad \frac{\mathrm{d}}{\mathrm{d}x}S_0^{\downarrow}(x) = -\sigma^{-1}(x) \tag{3.24}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}x}S_1^{\uparrow}(x) = \frac{\mathrm{d}}{\mathrm{d}x}S_1^{\downarrow}(x) = \frac{\sigma'(x)}{2\sigma(x)} - \frac{f(x)}{\sigma^2(x)}. \tag{3.25}$$

A full exploration of the possible behaviors of the solutions of (3.22) is beyond the scope of this article. We note, however, that when σ is a constant, the solutions

$$\phi^{\uparrow}(x) = \exp\left((2\lambda)^{\frac{1}{2}}\sigma^{-1}x - \sigma^{-2}\int_0^x f(z)\,\mathrm{d}z + \mathcal{O}(2\lambda)^{-\frac{1}{2}}\right) \tag{3.26}$$

and

$$\phi^{\downarrow}(x) = \exp\left(-(2\lambda)^{\frac{1}{2}}\sigma^{-1}x - \sigma^{-2}\int_0^x f(z)\,\mathrm{d}z + \mathcal{O}(2\lambda)^{-\frac{1}{2}}\right) \tag{3.27}$$

are consistent with (3.15) and (3.17).

4. Comparison of timestepping methods. In this section we describe two exponential-timestepping algorithms, based on the analysis of section 3. We also report on numerical experiments performed with exponential and fixed-step algorithms.

4.1. The exponential-Euler method with boundary test. The strategy of the first exponential-timestepping algorithm we have implemented is to approximate the process $\mathbf{X}$ at each time by a Brownian motion with constant drift, with parameters evaluated at the current position. Like the Euler method, the timestepping is exact, i.e., the statistics are exactly correct at the end of the timestep, when both $f(x)$ and $\sigma(x)$ are constants. The method produces updates and boundary tests according to (3.4), (3.7), and (3.8), with $\mu = f(\mathbf{X}_t)$ and $\epsilon = \sigma(\mathbf{X}_t)$.

At each step, two random variables are needed:

- a random variable, $\mathbf{u}$, uniformly distributed in $(0, 1)$;
- an exponentially distributed random variable, $\mathbf{p}$, generated as $-\log \mathbf{v}$, where $\mathbf{v}$ is uniformly distributed in $(0, 1)$ and independent of $\mathbf{u}$.

The increment $\mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t$ is given by (3.4):

$$\mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t = (\mathbf{N}_t - \mathbf{s}\mathbf{F}_t)^{-1}\mathbf{s}\,\mathbf{p}, \tag{4.1}$$

where

$$\mathbf{F}_t = \sigma(\mathbf{X}_t)^{-2} f(\mathbf{X}_t), \qquad \mathbf{N}_t = \left(\frac{2\lambda}{\sigma(\mathbf{X}_t)^2} + \mathbf{F}_t^2\right)^{\frac{1}{2}},$$

and

$$\mathbf{s} = \operatorname{sign}\left(\tfrac{1}{2}\left(1 + \mathbf{F}_t/\mathbf{N}_t\right) - \mathbf{u}\right). \tag{4.2}$$

After generating the value of $\mathbf{X}_{t+\boldsymbol{\delta t}}$, we perform the test for a boundary at $b > \mathbf{X}_t$ by generating a third random variable,

- $\mathbf{w}$, uniformly distributed in $(0, 1)$.

The boundary is deemed to have been reached if

$$\mathbf{X}_{t+\boldsymbol{\delta t}} > b \quad \text{or} \quad \mathbf{w} < \exp\left(-2\mathbf{N}_t(b - (\mathbf{X}_t \vee \mathbf{X}_{t+\boldsymbol{\delta t}}))\right). \tag{4.3}$$

A similar philosophy to that of the exponential-Euler method has been applied to the fixed-step Euler method. In the latter case, an "interpolating" process is defined as a constant-drift Brownian bridge in each time interval Δt [11]. The conditional exit probability, analogous to (3.7), is

$$\mathcal{P}[\mathbf{H}_b^{\mathbf{X}}(x) < \Delta t | \mathbf{X}_{\Delta t} = y] = \exp\left(-2\frac{(b-x)(b-y)}{\sigma^2(x)\Delta t}\right). \tag{4.4}$$

4.2. The exponential-V method with boundary test. The second new algorithm we have implemented is appropriate for additive noise problems and is based on the results of section 3.2. The potential function $V(x)$, defined in (3.16), is evaluated at each step.

Let

$$\mathbf{a} = \mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t. \tag{4.5}$$

For $x > 0$, the density of the random variable $\mathbf{a}$, (3.18), is

$$-\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{P}[\mathbf{a} > x] = N \exp\left(-\nu x + \epsilon^{-2}\left(V(\mathbf{X}_t + x) - V(\mathbf{X}_t)\right) + \mathcal{O}(\nu^{-1})\right). \tag{4.6}$$

We generate a random variable $\mathbf{a}^*$, with density approximating that of $\mathbf{a}$, as follows:

$$\mathbf{a}^* = \nu^{-1} F(-\log \mathbf{u}), \tag{4.7}$$

where $\mathbf{u}$ is uniformly distributed between 0 and 1. Let

$$R_{\mathbf{a}^*}(x) = -\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{P}[\mathbf{a}^* > x]. \tag{4.8}$$

When $F(x) = x$, $\mathbf{a}^*$ is exponentially distributed, i.e., $R_{\mathbf{a}^*}(x) = \nu \exp(-\nu x)$. More generally, the density of $\mathbf{a}^*$ can be expressed in terms of the inverse function $F^{-1}(x)$:

$$\begin{aligned}\mathcal{P}[\mathbf{a}^* > x] &= \mathcal{P}[F(-\log \mathbf{u}) > \nu x] \\ &= \mathcal{P}[-\log \mathbf{u} > F^{-1}(\nu x)] \\ &= \mathcal{P}[\mathbf{u} > \exp(-F^{-1}(\nu x))] \\ &= \exp(-F^{-1}(\nu x)). \qquad (4.9)\end{aligned}$$

Thus

$$\begin{aligned}R_{\mathbf{a}^*}(x) &= \nu G(\nu x) \exp(-F^{-1}(\nu x)) \\ &= \nu \exp\left(-F^{-1}(\nu x) + \log(G(\nu x))\right), \qquad (4.10)\end{aligned}$$

where

$$G(x) = \frac{\mathrm{d}}{\mathrm{d}x}F^{-1}(x).$$

In order to reproduce (4.6) when $\nu x = \mathcal{O}(1)$, we need $F^{-1}(\nu x) = \nu x + \epsilon^{-2}(V(\mathbf{X}_t + x) - V(\mathbf{X}_t)) + \mathcal{O}(\nu^{-1})$. We therefore expand the function $F(y)$ as follows:

$$F(y) = y + F_1(y/\nu) + \mathcal{O}(\nu^{-1}), \tag{4.11}$$

where $F_1(0) = 0$ and the function F_1 depends on the value of $\mathbf{X}_t$. Then

$$F^{-1}(z) = z - F_1(z/\nu) + \mathcal{O}(\nu^{-1}) \tag{4.12}$$

and

$$G(z) = 1 + \mathcal{O}(\nu^{-1}). \tag{4.13}$$

So

$$R_{\mathbf{a}^*}(x) = \nu \exp\left(-\nu x + F_1(x) + \mathcal{O}(\nu^{-1})\right). \tag{4.14}$$

Comparing with (3.18), we require $F_1(x) = -\epsilon^{-2}(V(\mathbf{X}_t + x) - V(\mathbf{X}_t))$ in order that (4.14) and (4.6) coincide. That is

$$\mathbf{a}^* = \nu^{-1}\left(\mathbf{p} - \epsilon^{-2}(V(\mathbf{X}_t + \nu^{-1}\mathbf{p}) - V(\mathbf{X}_t))\right). \tag{4.15}$$

The analysis for $x < 0$ is similar.

To generate the increment $\mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t$, we use two random variables:

- $\mathbf{u}$, uniformly distributed in $(0, 1)$;
- $\mathbf{p}$, exponentially distributed, generated as $-\log \mathbf{v}$, where $\mathbf{v}$ is uniformly distributed in $(0, 1)$ and independent of $\mathbf{u}$.

Then

$$\mathbf{X}_{t+\boldsymbol{\delta t}} - \mathbf{X}_t = \nu^{-1}\mathbf{s}\left(\mathbf{p} - \epsilon^{-2}\left(V(\mathbf{X}_t + \nu^{-1}\mathbf{s}\mathbf{p}) - V(\mathbf{X}_t)\right)\right), \tag{4.16}$$

where

$$\mathbf{s} = \operatorname{sign}\left(\tfrac{1}{2}\left(1 + \nu^{-1}\epsilon^{-2}f(\mathbf{X}_t)\right) - \mathbf{u}\right). \tag{4.17}$$

This procedure reproduces the density (3.18) in the limit $\nu^{-1} \to 0$.

After generating the value of $\mathbf{X}_{t+\boldsymbol{\delta t}}$, the test for a boundary at $b > \mathbf{X}_t$ is performed by generating a third random variable:

- $\mathbf{w}$, uniformly distributed in $(0, 1)$.

The boundary is deemed to have been reached if

$$\mathbf{X}_{t+\boldsymbol{\delta t}} > b \quad \text{or} \quad \mathbf{w} < \exp\left(-2\nu(b - (\mathbf{X}_t \vee \mathbf{X}_{t+\boldsymbol{\delta t}}))\right). \tag{4.18}$$

4.3. Numerical experiments: Double-well potential. We report on numerical experiments where our algorithms were applied to the additive noise problem ($\sigma(x) = \epsilon$) with $f(x) = -8x + 12x^2 - 4x^3$, corresponding to the potential $V(x)$ shown in Figure 4.1.

This process has a stationary density equal to $\hat{m}(x)$, where [14, 15, 17]

$$\hat{m}(x) = M^{-1}\exp\left(-2\epsilon^{-2}V(x)\right), \tag{4.19}$$

the constant M being chosen so that

$$\int_{-\infty}^{\infty} \hat{m}(z)\,\mathrm{d}z = 1. \tag{4.20}$$

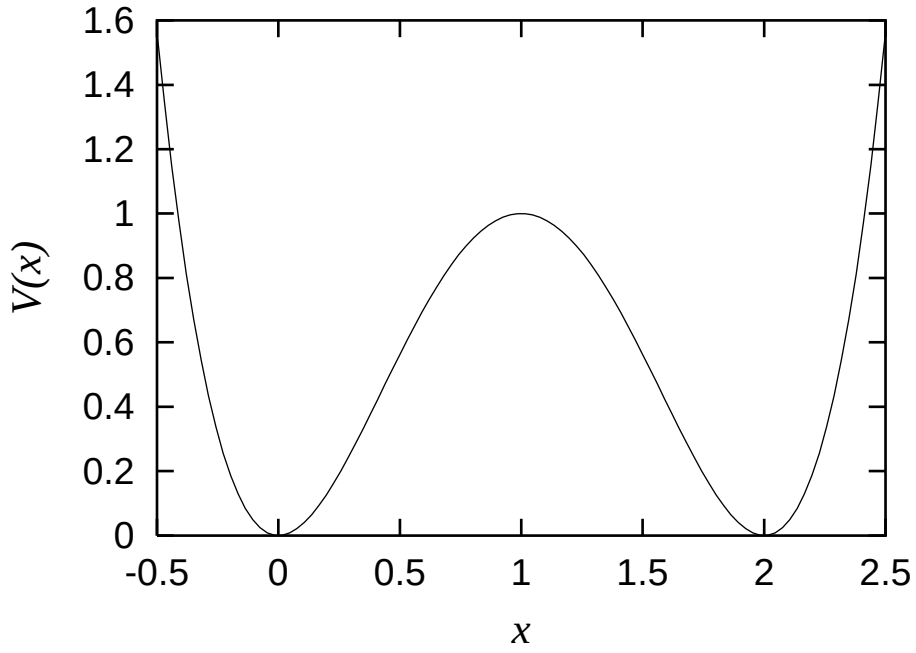

FIG. 4.1. *The potential function $V(x) = 4x^2 - 4x^3 + x^4$, used in the numerical experiments. We take $\mathbf{X}_0 = 0$ and measure the mean passage time to $b = 1$.*

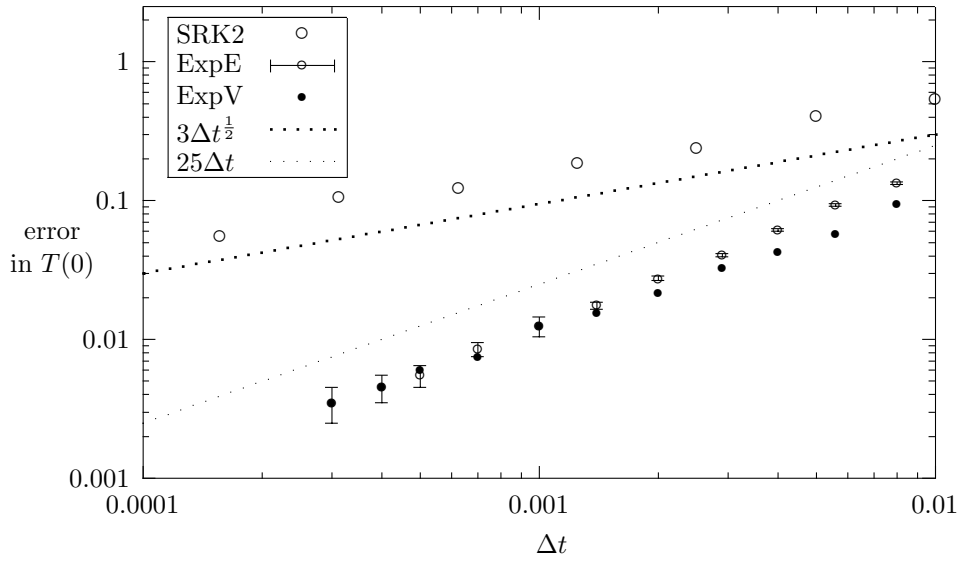

FIG. 4.2. *Error in numerically estimated mean escape time. Large empty circles: SRK2 method without boundary correction. Empty circles with error bars: exponential-Euler method with boundary correction. The horizontal axis is* λ^{-1}. *Filled circles: exponential-V method with boundary correction. The horizontal axis is* λ^{-1}. *The upper dotted line is proportional to* $\Delta t^{\frac{1}{2}}$ *and the lower is proportional to* Δt.

The quantity $\langle \mathbf{X}_t{}^2 \rangle$ therefore approaches a well-defined limit as $t \to \infty$. Angled brackets indicate mean over realizations. As a preliminary test, we ran many independent numerical realizations, under the various algorithms available to us, and took the mean squared value for $t = 10$. This mean over numerical realizations contains a statistical error, which decreases as more realizations are generated, and a systematic error that is an increasing function of Δt (fixed-step methods) or λ^{-1} (exponential methods). For the standard Euler method the systematic error was found to be proportional to Δt; for both the exponential-Euler and exponential-V methods, it is proportional to λ^{-1}. This is consistent, in all three cases, with convergence of (weak) order 1. Note that, for additive noise problems, weak order 2 convergence can be obtained using the stochastic second order Runge–Kutta (SRK2) method [1, 2, 16].

In the numerical experiments whose results are displayed in Figure 4.2, the quantity numerically measured is the first time that the process reaches the value $b = 1$ starting from $x = 0$. The exact value of this quantity is obtained as follows. Let

$$\mathbf{H}^{\mathbf{X}}_{a,b}(x) = \mathbf{H}^{\mathbf{X}}_{a}(x) \wedge \mathbf{H}^{\mathbf{X}}_{b}(x), \tag{4.21}$$

where $a < x < b$ and let $T(x) = \langle \mathbf{H}^{\mathbf{X}}_{a,b}(x) \rangle$. Then $T(x)$ satisfies [14, 15, 16]

$$\frac{1}{2}\epsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} T(x) + f(x) \frac{\mathrm{d}}{\mathrm{d}x} T(x) = -1 \tag{4.22}$$

with

$$T(a) = 0 \quad \text{and} \quad T(b) = 0. \tag{4.23}$$

Here we let $a \to -\infty$. The solution is [17]

$$T(x) = 2\epsilon^{-2} \int_{-\infty}^{x} \frac{\mathrm{d}y}{m(y)} \int_{y}^{b} m(z)\mathrm{d}z. \tag{4.24}$$

Without a boundary test, all of the methods we have used produce an error in the mean exit time proportional to $\Delta t^{\frac{1}{2}}$ [20, 21, 11]. As an illustration, in Figure 4.2, we plot the error in the mean escape time for $\epsilon = 1$, using the SRK2 method. The good accuracy that this method has in the timestepping per se is of no help in the evaluation of the exit time.

In Figure 4.2 we plot the systematic error in the mean exit time, taken over numerical realizations, under the exponential-Euler and exponential-V methods. Error bars are shown only in the second case for clarity. The total time elapsed after n exponential timesteps (with constant λ) is $n\lambda^{-1}$. Notice that the precise value of the elapsed time is not recorded, but that the error so introduced is statistical and not systematic.

In our numerical examples, the boundary test is responsible for improving the order of convergence from an error in the mean exit time proportional to $\Delta t^{\frac{1}{2}}$ to one proportional to Δt. We expect this to be true for a large class of examples, but we do not have a rigorous proof. Under fixed-step Euler timestepping, it has been shown that using the boundary test (4.4) improves the order of convergence from $\mathcal{O}(\Delta t^{\frac{1}{2}})$ to $\mathcal{O}(\Delta t)$ in evaluation of $\left\langle f(\mathbf{X}_t) | t < \mathbf{H}_b^{\mathbf{X}} \right\rangle$ for a class of functions $f(x)$ with support away from the boundary. Our own numerical tests using the fixed-step Euler method and (4.4) suggest that the convergence with $\mathcal{O}(\Delta t)$ also applies to the evaluation of the exit time. Similar improvements to the Euler method can be obtained by discretizing space as well as time [21]. For methods based on exponential timestepping, we hope that further study of the solutions of (2.4) will lead to methods of higher order, both in timestepping and the evaluation of exit times.

5. Conclusion. The characteristic of the numerical methods presented here is that values of the process $\mathbf{X}$ are generated at times separated by a random variable $\boldsymbol{\delta t}$, distributed as in (1.3). This choice permits an efficient scheme for problems involving a special value of the process, such as a boundary, because a simple boundary test can be performed after each update.

We have implemented two methods. The first is analogous to the usual Euler method for a fixed-duration timestep in that the drift and diffusion coefficients are evaluated using the values at the beginning of the timestep. The second method takes advantage of the existence of an analytical form for the potential function in additive noise problems. We have not given a rigorous proof of convergence for these methods, but we hope that analysis of the behavior of solutions of the ordinary differential equation (2.4) will lead to a simple general proof of weak convergence. The higher-dimensional analogue of (2.4) is the basis for work in progress on extensions of exponential timestepping methods to higher dimensions.

Appendix A. Normalization of the density of increments. The normalization factor, N, of the density (2.12) is given by

$$N = \left(\phi^{\downarrow}(x) \int_{-\infty}^{x} m(y)\phi^{\uparrow}(y)\,\mathrm{d}y + \phi^{\uparrow}(x) \int_{x}^{\infty} m(y)\phi^{\downarrow}(y)\,\mathrm{d}y \right)^{-1}. \tag{A.1}$$

It is at first sight a function of x. We show that it is in fact independent of x. Let

$$W(x) = \left(\phi^{\downarrow}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow} - \phi^{\uparrow}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\downarrow}\right). \tag{A.2}$$

Then, using (2.4)

$$\frac{\mathrm{d}W(x)}{\mathrm{d}x} = \left(\phi^{\downarrow}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi^{\uparrow} - \phi^{\uparrow}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi^{\downarrow}\right). \tag{A.3}$$

Now, multiplying (2.4) by $\phi^{\downarrow}(x)$ and by $\phi^{\uparrow}(x)$ yields

$$\frac{1}{2}\sigma^2(x)\frac{\mathrm{d}W(x)}{\mathrm{d}x} + f(x)W(x) = 0. \tag{A.4}$$

Thus

$$W(x) = \frac{2}{\sigma^2(x)}\frac{A}{m(x)}, \tag{A.5}$$

where $m(x)$ is defined in (2.13) and A is a constant.

We rewrite (2.4) as follows:

$$\mathcal{L}\phi(x) = \lambda\phi(x), \tag{A.6}$$

where

$$\mathcal{L}\phi^{\uparrow}(x) = \frac{A}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x)\right). \tag{A.7}$$

Rearranging (A.6) gives

$$A\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x)\right) = \lambda m(x)\phi^{\uparrow}(x). \tag{A.8}$$

Integrating (A.8) yields

$$\frac{A}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x) = \lambda\int_{-\infty}^{x} m(y)\phi^{\uparrow}(y)\,\mathrm{d}y. \tag{A.9}$$

Similarly, we obtain

$$-\frac{A}{W(x)}\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\downarrow}(x) = \lambda\int_{x}^{\infty} m(y)\phi^{\downarrow}(y)\,\mathrm{d}y. \tag{A.10}$$

Using (A.9) and (A.10), we find that

$$N^{-1} = \frac{1}{\lambda}\frac{A}{W(x)}\left(\phi^{\downarrow}(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\uparrow}(x) - \phi^{\uparrow}(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi^{\downarrow}(x)\right) \tag{A.11}$$

$$= \frac{A}{\lambda}. \tag{A.12}$$

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