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Efficient Numerical Solution of Stochastic Differential Equations Using Exponential Timestepping

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We present an exact timestepping method for Brownian motion that does not require Gaussian random variables to be generated. Time is incremented in steps that are exponentially-distributed random variables; boundaries can be explicitly accounted for at each timestep. The method is illustrated by numerical solution of a system of diffusing particles.

KEY WORDS: Stochastic calculus; stochastic algorithms; Wiener process; diffusion with boundaries.

1. INTRODUCTION

Numerical methods that are in common use[1–4] for solving stochastic differential equations have a timestep of fixed length, perhaps divided up into intermediate timesteps and dynamically adapted. However, it is also possible to have a timestep whose length is a random variable.[5, 6] We present a method where *the timestep is a random variable with an exponential distribution.*

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The simplest case of a stochastic process is the Wiener process. An exact update for this process under a fixed timestep method requires generation of a Gaussian random variable. Under exponential timestepping, an exact new value is generated at a time incremented by $\boldsymbol{\delta t}$, where $\mathscr{P}[\boldsymbol{\delta t} > t] = \exp(-\lambda t)$, using an exponentially distributed random variable. The latter can be generated as minus the logarithm of a uniformly distributed random variable, at less computational cost than that involved in generating a Gaussian random variable. The price to be paid is uncertainty as to the value of the incremented time.

Exponential timestepping has an advantage over fixed-timestep methods when the stochastic differential equation models a diffusing particle in a space with special points, such as boundaries or other particles. In such situations, one must deal with the possibility that, even though the process may be on the same side of a boundary at time t and at time $t + \Delta t$, there is a finite probability that the boundary was hit at some intermediate time.[7] This probability can be calculated exactly in many cases when Δt is exponentially distributed, using methods from excursion theory.[8–15] Another appealing feature is that the density of the position at the end of the exponential timestep for the subset of paths that hit the boundary before the end of the timestep is the same *as if the timestep had started at the boundary*.

Each path of a Markov stochastic process that starts at the origin can be divided up into a series of excursions starting and ending at the origin.[8–15] Successive excursions are independent. The task of the excursion theorist is to assign relative probabilities or "rates" to sets of excursions: they can, for example, be classified according to the maximum distance of the process from the origin during the excursion. A timestep that is an exponentially-distributed random variable can be naturally incorporated into these calculations by including a constant probability per unit time that the path is "marked." Similarly, absorbing boundaries can be included by specifying that the path is "killed" if a certain point is reached during an excursion.

Section 2 is devoted to definitions and basic results for the Wiener process. In Section 3, we describe the implementation of exponential timestepping for the Wiener process: we generate an exponential and a ± 1-distributed random variable at each timestep. In the presence of a boundary, the possibility of hitting the boundary is exactly taken into account by generating, in addition, a uniformly-distributed random variable at each timestep Section 3 also contains the example of a Brownian particle diffusing between two boundaries that are themselves diffusing. We dynamically vary the parameter controlling the mean value of the timestep. In Section 4, we conclude. Extensions of the method of exponential timestepping to more general processes with continuous paths are being developed.[17]

2. DEFINITIONS

2.1. Wiener Process

The process $\mathbf{W}_t$, for which

$$\mathbf{W}_0 = 0, \qquad \langle \mathbf{W}_t \mathbf{W}_s \rangle = \min(t, s) \tag{1}$$

is usually called the Wiener process (or standard Brownian motion). For any time t and *fixed* timestep Δt, the increment $\mathbf{W}_{t+\Delta t} - \mathbf{W}_t$ is a Gaussian random variable with mean 0 and variance Δt.

Let $\boldsymbol{\delta t}$ be exponentially distributed:

$$\mathscr{P}[\boldsymbol{\delta t} > t] = \exp(-\lambda t) \tag{2}$$

Then

$$\mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} > x] = \int_0^\infty \lambda \exp(-\lambda t) \frac{1}{2} \left(1 - \operatorname{erf}\left(\frac{x}{\sqrt{2t}}\right)\right) \mathrm{d}t \tag{3}$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} \mathrm{d}y \tag{4}$$

Thus $\mathbf{W}_{\boldsymbol{\delta t}}$ has a symmetric exponential, rather than Gaussian, distribution:

$$\mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} > x] = \mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} < -x] = \tfrac{1}{2} e^{-\nu x} \tag{5}$$

where

$$\nu = \sqrt{2\lambda} \tag{6}$$

2.2. Passage Time

The passage time $\mathbf{H}_b$ is defined by

$$\mathbf{H}_b = \inf\{t > 0 : \mathbf{W}_t = b\} \tag{7}$$

This quantity can be directly calculated, using the up-down symmetry of Wiener increments.[10] Let $t > 0$. Then

$$\mathscr{P}[\mathbf{H}_b < t] = \mathscr{P}[\mathbf{H}_b < t, \mathbf{W}_t < b] + \mathscr{P}[\mathbf{H}_b < t, \mathbf{W}_t > b] = 2\mathscr{P}[\mathbf{W}_t > b]$$
$$= \left(\frac{2}{\pi t}\right)^{1/2} \int_b^\infty e^{-y^2/2t} \mathrm{d}y = 1 - \operatorname{erf}\left(\frac{b}{\sqrt{2t}}\right) \tag{8}$$

The density of $\mathbf{H}_b$,

$$R(t) = \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{P}[\mathbf{H}_b < t] \tag{9}$$

is obtained by differentiating (8) with respect to t and using integration by parts:

$$R(t) = \frac{|b|}{\sqrt{2\pi t^3}}\, e^{-b^2/2t} \tag{10}$$

2.3. Boundaries

Consider the subset of paths for which $\mathbf{H}_b < \boldsymbol{\delta t}$. For an event Θ, let

$$\mathscr{S}[\Theta] = \mathscr{P}[\Theta \mid \mathbf{H}_b < \boldsymbol{\delta t}] \tag{11}$$

For example,

$$\mathscr{S}[\mathbf{W}_{\boldsymbol{\delta t}} < 0] = \mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} < 0 \mid \mathbf{H}_b < \boldsymbol{\delta t}] = \frac{\mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} < 0, \mathbf{H}_b < \boldsymbol{\delta t}]}{\mathscr{P}[\mathbf{H}_b < \boldsymbol{\delta t}]} \tag{12}$$

For the complementary event, let

$$\mathscr{Q}[\Theta] = \mathscr{P}[\Theta \mid \mathbf{H}_b \geqslant \boldsymbol{\delta t}] \tag{13}$$

The probability that $\mathbf{H}_b < \boldsymbol{\delta t}$ can be obtained by direct integration over the density (10):

$$\begin{aligned}\mathscr{P}[\mathbf{H}_b < \boldsymbol{\delta t}] &= \frac{b}{\sqrt{2\pi}} \int_0^\infty t^{-3/2} \exp\left(-\frac{b^2}{2t} - \lambda t\right) \mathrm{d}t \\ &= e^{-\nu b}\end{aligned} \tag{14}$$

Similarly, the density of $\mathbf{W}_{\boldsymbol{\delta t}}$ conditioned on having hit b is given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathscr{S}[\mathbf{W}_{\boldsymbol{\delta t}} < x] = \frac{1}{2}\,\nu \exp(-\nu\,|b - x|) \tag{15}$$

Note that (15) is the same density as that after an unconditioned timestep started at the boundary b.

3. EXPONENTIAL TIMESTEPPING FOR THE WIENER PROCESS

To generate an increment of the Wiener process under exponential timestepping, two random variables are required. The first, **s**, takes the values $+1$ or -1 with equal probability. The second, **p**, is exponentially distributed:

$$\mathscr{P}[\mathbf{p} > x] = \exp(-x) \tag{16}$$

Given the value of $\mathbf{W}_t$, the value of $\mathbf{W}_{t+\boldsymbol{\delta t}}$ is given by

$$\mathbf{W}_{t+\boldsymbol{\delta t}} = \mathbf{W}_t + \nu^{-1}\mathbf{sp} \tag{17}$$

Thus the density of the random variable $\mathbf{W}_{t+\boldsymbol{\delta t}} - \mathbf{W}_t$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathscr{P}[\mathbf{W}_{t+\boldsymbol{\delta t}} - \mathbf{W}_t < x] = \frac{1}{2}\nu \exp(-\nu\,|x|) \tag{18}$$

as required by (5). The value of $\mathbf{W}_{t+\boldsymbol{\delta t}}$ thus produced is exact in distribution. However, the exact value of $\boldsymbol{\delta t}$ at each timestep is not recorded. Note that

$$\langle \boldsymbol{\delta t} \rangle = \frac{1}{\lambda} \tag{19}$$

so that the elapsed time after N timesteps is a random variable with mean N/λ.

3.1. Exponential Timestepping with a Boundary

Suppose we are interested in the statistics of paths run until they hit a boundary at $b > 0$. The simplest way to ascertain the hitting time is to increment the process using either standard or exponential timestepping, producing values $\mathbf{X}_{t_0}, \mathbf{X}_{t_1}, \mathbf{X}_{t_2}, \ldots$, until $\mathbf{X}_{t_i} > b$ at some t_i. However, large errors result in realizations for which a boundary is hit within an interval (t_i, t_{i+1}), although both $\mathbf{X}_{t_i} < b$ and $\mathbf{X}_{t_{i+1}} < b$. The discretization represented in Fig. 1, for example, does not detect the first crossing of the dotted line, although the timestepping itself is exact. Under exponential timestepping, the possibility that the numerical method misses a crossing and thus seriously overestimates the first hitting time can be explicitly excluded.

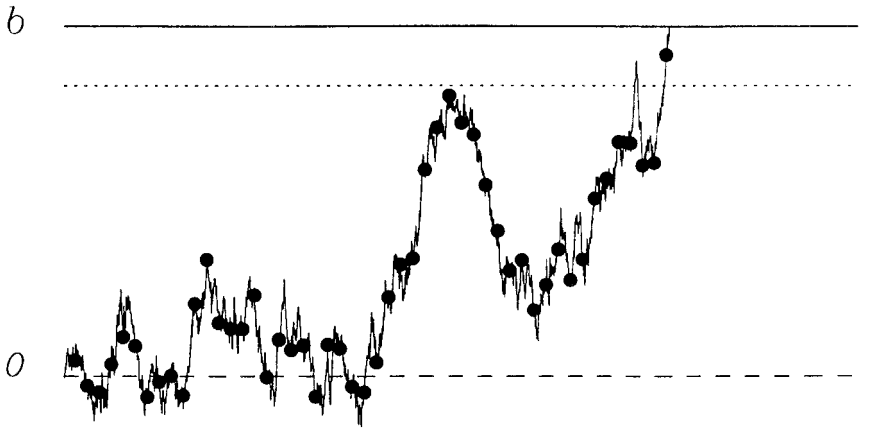

Fig. 1. Wiener path with an absorbing boundary at b. The dots are equally-spaced in time, representing a standard discretization.

Let $\mathbf{W}_{\boldsymbol{\delta t}} = z$. Then the probability that the boundary at b has been hit between $t = 0$ and $t = \boldsymbol{\delta t}$ is given by

$$\mathscr{P}[\mathbf{H}_b < \boldsymbol{\delta t} \mid \mathbf{W}_{\boldsymbol{\delta t}} = z] = \frac{\mathscr{P}[\mathbf{H}_b < \boldsymbol{\delta t}, \mathbf{W}_{\boldsymbol{\delta t}} = z]}{\mathscr{P}[\mathbf{W}_{\boldsymbol{\delta t}} = z]}$$

$$= \begin{cases} 1 & z \geqslant b \\ e^{-2v(b-z)} & 0 < z < b \\ e^{-2vb} & z \leqslant 0 \end{cases} \tag{20}$$

Exponential timestepping in the presence of a boundary therefore proceeds as follows:

(i) Generate an increment according to (17).

(ii) Generate a uniformly-distributed random variable $\mathbf{u}$. Let the positions before and after the increment (i) be x and z. *A boundary at* $b > x$ *is deemed to have been hit during the timestep if* $\mathbf{u} < P$ where

$$P = \begin{cases} 1 & z \geqslant b \\ e^{-2v(b-z)} & x \leqslant z < b \\ e^{-2v(b-x)} & z < x \end{cases} \tag{21}$$

A process that evolves for a time that is an exponentially-distributed random variable is equivalent to a process that is run with a constant

probability per unit time of being "marked."[8–14] One consequence of this is that the statistics of the fraction of paths that hit b before the end of the timestep (and are allowed to continue) are the same as the statistics that would be found if the process were run for an exponentially-distributed time starting at b (see (15)). On the other hand, the density defined by

$$R^c(x) = \frac{\mathrm{d}}{\mathrm{d}x}\,\mathcal{Q}[\mathbf{W}_{\delta t} < x] \tag{22}$$

is given by

$$R^c(x) = \frac{\nu}{2}\,(e^{-\nu|x|} - e^{-\nu b}e^{-\nu(b-x)})(1 - e^{-\nu b})^{-1} \qquad x < b \tag{23}$$

3.2. Exponential Timestepping with Diffusing Boundaries

We have introduced exponential timestepping for Wiener processes with constant boundaries. We now illustrate the use of the exponential timestepping algorithm in the following context. A test particle whose paths are those of a Wiener process diffuses, starting at the origin, between upper and lower boundaries that are themselves following Wiener paths. The initial positions of the boundaries are b and $-a$. Which boundary is hit first? We show that the exponential timestepping algorithm resolves the small difference between the cases of diffusing and non-diffusing boundaries. The algorithm for this case is no longer exact: at each timestep we correct only for the closest boundary.

The distance between two Brownian particles evolves with twice the mean-square displacement of a Wiener process. Thus, to ascertain whether the test particle has hit the closest boundary, we implement the test (21) with the replacement $\nu \to \nu/\sqrt{2}$. In addition, we have found that dynamically adapting the value of the parameter ν that controls the mean length of the exponential timestep leads to an efficient algorithm.

Before presenting numerical comparisons, we first calculate the probability that the upper boundary is hit before the lower boundary. Let $\mathbf{V}_t$ and $\mathbf{U}_t$ be Wiener processes, independent of each other and of $\mathbf{W}_t$, with

$$\begin{aligned} \mathbf{U}_0 &= b \\ \mathbf{V}_0 &= -a \end{aligned} \tag{24}$$

Let $\mathbf{H}^*_b = \inf\{t > 0 : \mathbf{W}_t = \mathbf{U}_t\}$, $\mathbf{H}^*_{-a} = \inf\{t > 0 : \mathbf{W}_t = \mathbf{V}_t\}$ and $\mathbf{t}^* = \min(\mathbf{H}^*_b, \mathbf{H}^*_{-a})$.

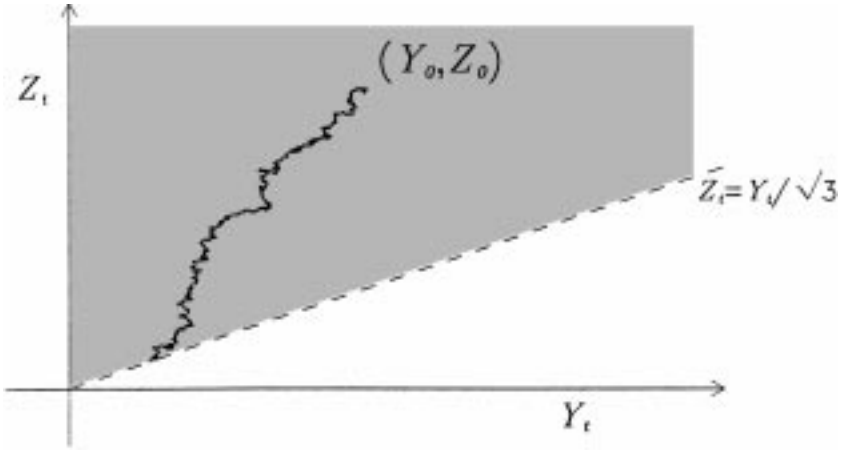

Fig. 2. The density of $\mathbf{t}^*$ is equal to that of the first exit time of a two-dimensional Brownian motion from the shaded region.

Now

$$\langle (\mathbf{U}_t - \mathbf{W}_t)(\mathbf{W}_t - \mathbf{V}_t) \rangle = -t \tag{25}$$

We change variables to a two-dimensional diffusion with *independent* components, defining two new Wiener processes $\mathbf{Y}_t$ and $\mathbf{Z}_t$ and setting

$$\begin{aligned} \mathbf{U}_t - \mathbf{W}_t &= \sqrt{2}\,\mathbf{Y}_t \\ \mathbf{W}_t - \mathbf{V}_t &= \frac{1}{\sqrt{2}}(-\mathbf{Y}_t + \sqrt{3}\,\mathbf{Z}_t) \end{aligned} \tag{26}$$

The density of $\mathbf{t}^*$ is the same as the density of first exit of Brownian motion from the domain shown in Fig. 2.

Let $\mathbf{R}_0 = (\mathbf{Y}_0^2 + \mathbf{Z}_0^2)^{1/2}$, $\Theta_0 = \operatorname{atan}(\mathbf{Z}_0/\mathbf{Y}_0)$ and

$$h(r, \phi) = \mathscr{P}[\mathbf{H}_b^* < \mathbf{H}_{-a}^* \mid \mathbf{R}_0 = r, \Theta_0 = \phi] \tag{27}$$

Then $h(r, \phi)$ is defined on $r \geqslant 0$, $\pi/6 \leqslant \phi \leqslant \pi/2$ and satisfies

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \right) h(r, \phi) = 0 \tag{28}$$

with the boundary conditions

$$h\left(r, \frac{\pi}{6}\right) = 0, \qquad h\left(r, \frac{\pi}{2}\right) = 1 \tag{29}$$

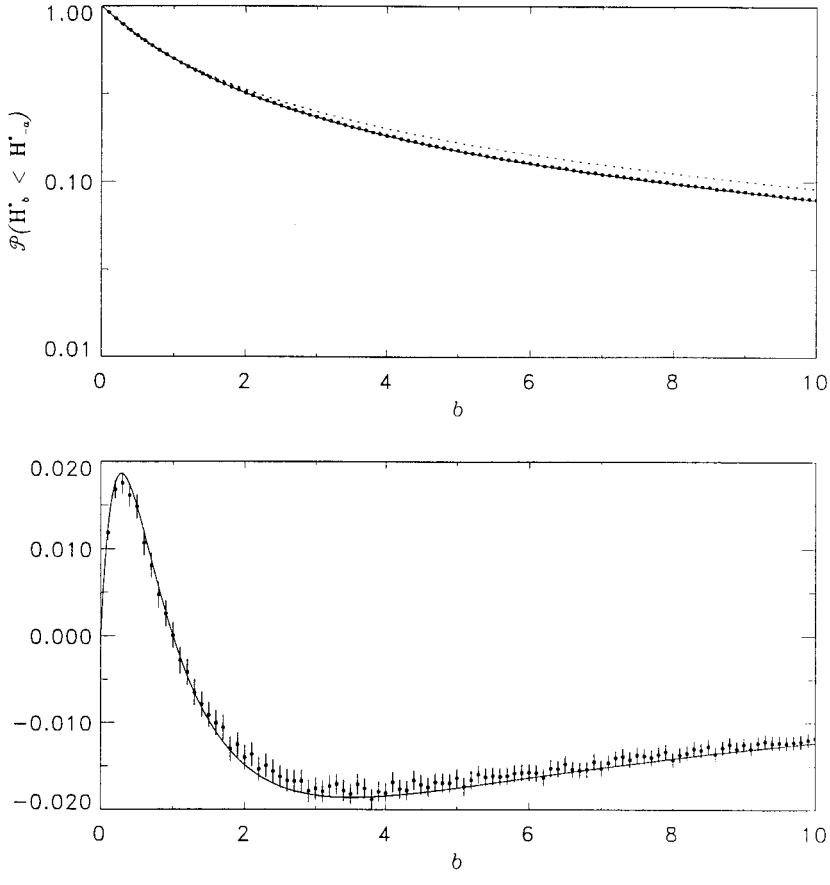

Fig. 3. Numerical results (dots with error bars) are compared with exact expressions (solid lines) in both graphs. The top graph plots the probability that the upper boundary is hit before the lower boundary when both are diffusing, versus the initial position of the upper boundary, b. The lower boundary has initial condition $-a = -1$. Also shown in the top graph is (33), the corresponding probability when the boundaries are fixed at b and $-a$ (dotted line). The bottom graph plots the difference between the cases of diffusing and fixed boundaries. The numerical results shown were obtained using exponential timestepping with boundary correction; the parameter v was dynamically adapted according to (34), with $\bar{v} = 20$.

The solution of (28) with (29) is simply

$$h(r, \phi) = \frac{3}{\pi}\left(\phi - \frac{\pi}{6}\right) \tag{30}$$

The initial conditions (24) correspond to

$$\begin{aligned} \mathbf{Y}_0 &= \frac{1}{\sqrt{2}} b \\ \mathbf{Z}_0 &= (2a + b)/\sqrt{6} \end{aligned} \tag{31}$$

In Fig. 3 we compare

$$\mathscr{P}[\mathbf{H}_b^* < \mathbf{H}_{-a}^*] = \frac{3}{\pi}\left(\operatorname{atan}\left(\frac{2a+b}{\sqrt{3b}}\right) - \frac{\pi}{6}\right) \tag{32}$$

with numerical results using the exponential timestepping algorithm and with the corresponding analytical result from the case where the upper and lower boundaries are fixed:

$$\mathscr{P}[\mathbf{H}_b < \mathbf{H}_{-a}] = \frac{a}{a+b} \tag{33}$$

The numerical results shown were obtained with the value of v chosen at each timestep according to

$$v = \bar{v}/(\mathbf{U}_t - \mathbf{V}_t) \tag{34}$$

where $\bar{v}$ is constant.

In Fig. 4, we plot the error in the numerically-measured fraction of paths hitting the upper boundary using exponential and Gaussian timestepping. The latter was performed with a fixed timestep $\Delta t = 0.001$ and no boundary correction was attempted. It produced a larger statistical error because, from the same amount of computer time, fewer realizations were obtained due to the cost of generating Gaussian random variables. Thus, in addition to being more accurate, exponential timestepping is more rapid for this problem.

In Fig. 5, we compare a histogram of values of the first time of a collision, generated using exponential timestepping, with the exact density of $\mathbf{t}^*$. Let

$$R^*(t) = \frac{d}{dt}\mathscr{P}[\mathbf{t}^* < t] \tag{35}$$

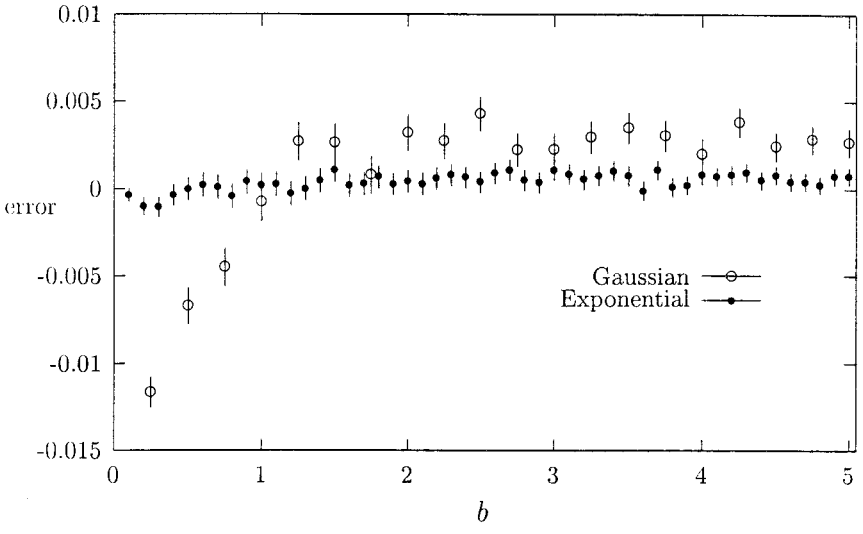

Fig. 4. The difference between the exact result (32) the numerically-measured fraction of paths hitting the upper boundary is plotted versus the initial position of the upper boundary, b. Gaussian timestepping was performed with $\Delta t = 0.001$; exponential timestepping was carried out with boundary correction and v varied according to (34), with $\bar{v} = 25$.

Then[16]

$$R^*(t) = \frac{1}{2}\frac{1}{\sqrt{\pi t^3}}\left(be^{-b^2/4t} + ae^{-a^2/4t} - (b+a)\, e^{-(b+a)^2/4t}\right) \tag{36}$$

The numerical histogram and the exact solution (36) are almost indistinguishable. Also shown is the density of the first exit time for the case of fixed boundaries.

4. CONCLUSION

The simplest method for numerical generation of paths approximating those of a continuous stochastic process is the Euler method. With a fixed timestep Δt, two increments are added at each update: a deterministic increment proportional to Δt and a mean-zero Gaussian random variable with standard deviation proportional to $\Delta t^{1/2}$. In this work, we implement the unconventional method of taking each timestep as a random variable: instead of a fixed timestep Δt, an exponentially-distributed timestep $\boldsymbol{\delta t}$ is used, with mean length λ^{-1}. The random increment at each timestep is now

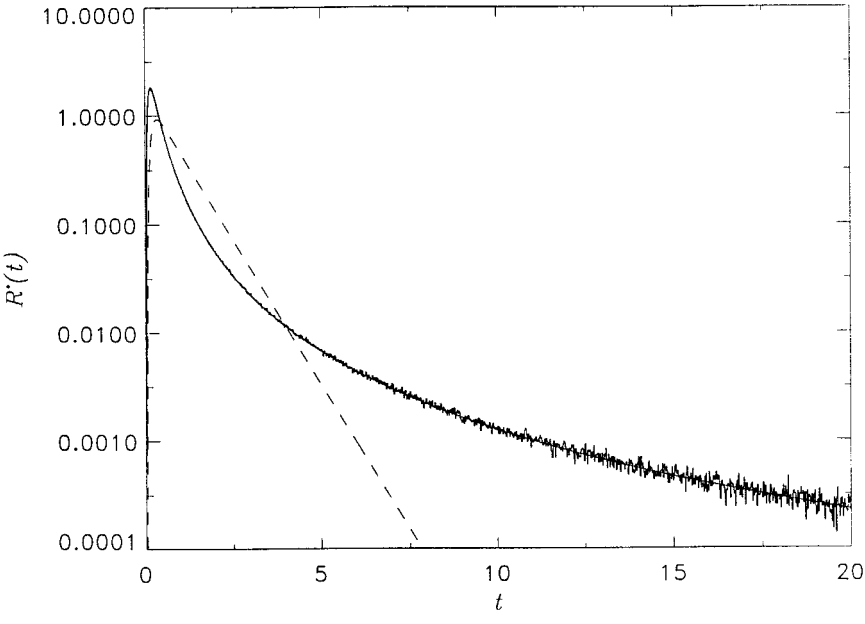

Fig. 5. The density of the first exit time for diffusing boundaries, (36), is compared with a histogram of numerical values, compiled using the exponential timestepping algorithm. The parameters in (36) are $a = b = 1$. Numerical values are N/λ where N is the number of timesteps before the first collision is recorded; each numerical realization was generated with $v = 40$. The agreement is such that (36), shown as a solid line, is almost invisible beneath the histogram. The dotted line, for comparison, is the density of the exit time for fixed boundaries at ± 1.

symmetric exponential with a factor of $\lambda^{1/2}$ in the exponent. In this work we restrict ourselves to the Wiener process, where the deterministic increment is zero at every timestep.

We believe that this method is likely to be efficient in the study of the diffusion of a collection of interacting point particles on a line, and this topic will be the subject of a future article.

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