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Monte Carlo simulation of diffusion in a spatially nonhomogeneous medium: A biased random walk on an asymmetrical lattice

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Abstract

Monte Carlo (MC) simulation of diffusion processes has proved to be a powerful and valuable adjunct to deterministic solutions of the diffusion equation. In its simplest one-dimensional implementation, a particle is stepped to left or right, with equal probability, a distance $\sqrt{2D\Delta t}$ where D is the diffusion coefficient and Δt is the timestep. This gives accurate results if D is constant, but in the case where D is spatially dependent a systematic error occurs, as shown by comparing MC averages with deterministic solutions. Furthermore, this error does not reduce when the timestep Δt is reduced. We show that the results can be reconciled by altering both the MC stepsize and stepping probability, and give simple formulas for the correction terms that are also applicable in higher dimensions. This supplements our previous work on corrections to the Gaussian-step MC method [J. Comput. Phys. 198 (2004) 65].

Keywords: Monte Carlo; Diffusion; Stochastic modelling; Random walk

1. Introduction

Monte Carlo (MC) simulation has proved a valuable tool for investigating processes involving the diffusion of substances. In particular, in has been used in neurophysiology to study the action of neurotransmitters [1–4,8] and more recently the function of calcium ions (Ca^{2+}) in initiating and modifying synaptic function [5,6,10,17].

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For the case of a constant diffusion coefficient $D = D_0$ there are two main ways of implementing MC diffusion. The simplest is to use a constant stepsize $L_0 = \sqrt{2D_0\Delta t}$ and step to the right or left with equal probability. (This is for diffusion in one dimension; it is easily extended to higher dimensions.) This is the approach taken by, for example [12,15,16,18]. Another method is to choose the stepsize from a Gaussian distribution; the step length is now $L_0 = \sqrt{2D_0\Delta t}\zeta$ where ζ is a standard normal deviate, that is, a number chosen at random from a Gaussian distribution with mean 0 and standard deviation 1. In this case, L_0 can be of either sign so it is not necessary to choose a direction. Examples of this approach can be found in [1–6,8].

In each case, the 'obvious' extension of these methods to the nonhomogeneous case would seem to be to replace D_0 by $D(x)$ in each formula. However, this turns out to introduce a systematic error (as measured by the difference between the average of a number of MC simulations and the deterministic solution of the diffusion equation); furthermore, this error does not decrease when the timestep Δt is reduced, even to very small values. We first became aware of this problem when attempting to reproduce Ca^{2+} diffusion results reported by Matveev et al. [14]. These authors used a diffusion coefficient that increased rapidly over a short distance (Fig. 1(a)) and solved the diffusion equation by a finite difference method. Our investigation of the discrepancy between the MC and deterministic results led to the development of a systematic method for calculating corrections to the Gaussian steplength [9]. It was also mentioned [9] that the alternative method of taking fixed steps to right or left suffered from the same problem, and for the same reason, namely that in the variable D case there is an inherent bias in the steplength that cannot be overcome by taking a shorter time interval since this simply increases the required number of steps and the total error remains the same. However, no method was given for correcting the fixed-step case and it is the purpose of this present work

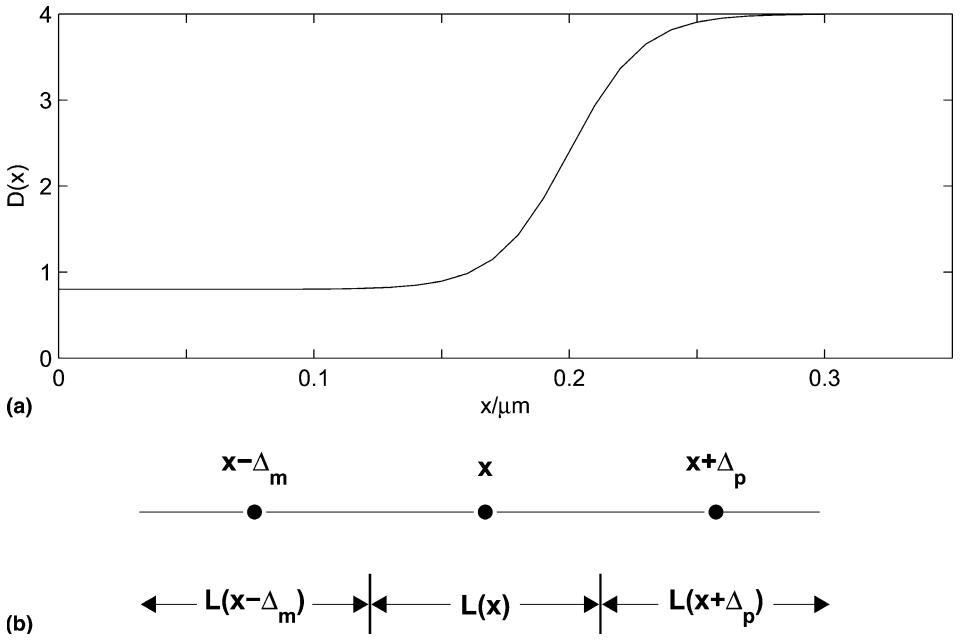

Fig. 1. (a) The spatially varying diffusion coefficient used in [14]. It is given by (see also the web site http://mrb.niddk.nih.gov/matveev) $D(x) = \widehat{D}[1 - 0.8u(x)]$, where $u(x) = \frac{1}{2}\{\tanh[A(b-x)] + 1\}$. The parameters are $\widehat{D} = 4\ \mu m^2\ s^{-1}$, $A = 35\ \mu m^{-1}$ and $b = 0.2\ \mu m$. (b) The lattice used in the one-dimensional random walk. $L(x) = \sqrt{2D(x)\Delta t}$ is the uncorrected steplength. The corrected steplengths, Δ_p and Δ_m, are the averages of $L(x)$ evaluated at the endpoints and are given implicitly by Eqs. (1).

to provide one. It turns out that both the steplength and the probability of stepping to left or right must be modified in order to provide a solution.

Investigation of the relation between diffusion and random walks goes back to the classic work of Einstein [7]. One of the first authors to draw explicit attention to the relation between random walks on a lattice and diffusion was Kac [11]. An elementary account of some of the main ideas can be found in the text by MacKeown [13]; a more comprehensive treatment is by van Kampen [19]. However, none of these works treat the present case of diffusion with a spatially varying diffusion coefficient.

2. Theory

2.1. The lattice

For a random walk starting at x, the lattice points to the right and to the left have coordinates $x + \Delta_p(x)$ and $x - \Delta_m(x)$, respectively, where $\Delta_p(x)$ and $\Delta_m(x)$ are defined implicitly by the equations

$$\Delta_p(x) = \frac{1}{2}[L(x) + L(x + \Delta_p(x))], \quad \Delta_m(x) = \frac{1}{2}[L(x - \Delta_m(x)) + L(x)], \tag{1}$$

where

$$L(x) \equiv \sqrt{2D(x)\Delta t}, \tag{2}$$

as illustrated in Fig. 1(b). With these choices for Δ_p and Δ_m the random walk stays precisely on the lattice, since each step (to right or left) is the average of $L(x)$ evaluated at the endpoints of the step; explicitly, $\Delta_m(x + \Delta_p(x)) = \Delta_p(x)$ and $\Delta_p(x - \Delta_m(x)) = \Delta_m(x)$. In the special case of a linearly varying diffusion coefficient

$$D(x) = D_0(1 + \alpha x), \tag{3}$$

where D_0 and α are constants, Eqs. (1) can be solved exactly to give

$$\Delta_p(x) = \sqrt{2D_0(1 + \alpha x)\Delta t} + \frac{1}{2}\alpha D_0 \Delta t, \quad \Delta_m(x) = \sqrt{2D_0(1 + \alpha x)\Delta t} - \frac{1}{2}\alpha D_0 \Delta t. \tag{4}$$

However, in general an exact solution is not possible (or even desirable, since we are only interested in finding a correction to the usual steplength) so an approximation must be used. This means that although the lattice is still fixed locally, in the sense that a particle currently at point x can only move to $x + \Delta_p$ or $x - \Delta_m$ at the next timestep, it is not fixed globally and eventually all positions on the line will be visited.

The first-order corrections to the steplengths can be found from Taylor expansions of Eqs. (1). Since $L(x) = \mathcal{O}(\sqrt{\Delta t})$,

$$\Delta_p(x) = L + \frac{1}{2}LL' + \mathcal{O}((\Delta t)^{3/2}), \quad \Delta_m(x) = L - \frac{1}{2}LL' + \mathcal{O}((\Delta t)^{3/2}), \tag{5}$$

where $L \equiv L(x)$ and $L' \equiv \mathrm{d}L(x)/\mathrm{d}x$.

2.2. Diffusion

Let $T_r(x)$ be the probability that a particle at position x moves to the right at the next time step and let $T_\ell(x)$ be the corresponding probability that it moves to the left, so that

$$T_r(x) + T_\ell(x) = 1. \tag{6}$$

If $p(x, t)$ is the probability that a particle is at position x at time t, then

$$p(x,t+\Delta t) = p(x+\Delta_p,t)T_\ell(x+\Delta_p) + p(x-\Delta_m,t)T_\mathrm{r}(x-\Delta_m), \tag{7}$$

where $\Delta_p \equiv \Delta_p(x)$ and $\Delta_m \equiv \Delta_m(x)$. If we now consider a large number of particles moving independently then the average number, $N(x,t)$, at point x and time t, will satisfy

$$N(x,t+\Delta t) = N(x+\Delta_p,t)T_\ell(x+\Delta_p) + N(x-\Delta_m,t)T_\mathrm{r}(x-\Delta_m). \tag{8}$$

The concentration of particles at point x at time t is

$$c(x,t) = N(x,t)/L(x). \tag{9}$$

(Note that division by $L(x)$ is important, since the lattice spacing varies with position.) The time rate of change of concentration at point x is

$$\frac{\partial c}{\partial t} = \lim_{\Delta t\to 0}\frac{c(x,t+\Delta t)-c(x,t)}{\Delta t} = \lim_{\Delta t\to 0}\frac{1}{L(x)}\frac{N(x,t+\Delta t)-N(x,t)}{\Delta t}. \tag{10}$$

Using Eq. (8) this can be written as

$$\frac{\partial c}{\partial t} = \lim_{\Delta t\to 0}\frac{1}{L(x)}\frac{1}{\Delta t}\left[L(x+\Delta_p)c(x+\Delta_p,t)T_\ell(x+\Delta_p) + L(x-\Delta_m)c(x-\Delta_m,t)T_\mathrm{r}(x-\Delta_m) - L(x)c(x,t)\right]. \tag{11}$$

We now use the Taylor expansions

$$c(x+\Delta_p) = c(x,t) + \Delta_p\frac{\partial c}{\partial x} + \frac{1}{2}\Delta_p^2\frac{\partial^2 c}{\partial x^2} + \mathcal{O}((\Delta t)^{3/2}), \tag{12}$$

$$c(x-\Delta_m) = c(x,t) - \Delta_m\frac{\partial c}{\partial x} + \frac{1}{2}\Delta_m^2\frac{\partial^2 c}{\partial x^2} + \mathcal{O}((\Delta t)^{3/2}), \tag{13}$$

to write Eq. (11) as

$$\begin{aligned}\frac{\partial c}{\partial t} = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\Bigg[&[R_p(x)T_\ell(x+\Delta_p) + R_m(x)T_\mathrm{r}(x-\Delta_m) - 1]c(x,t)\\ &+ [R_p(x)\Delta_p T_\ell(x+\Delta_p) - R_m(x)\Delta_m T_\mathrm{r}(x-\Delta_m)]\frac{\partial c}{\partial x}\\ &+ \frac{1}{2}[R_p(x)\Delta_p^2 T_\ell(x+\Delta_p) + R_m(x)\Delta_m^2 T_\mathrm{r}(x-\Delta_m)]\frac{\partial^2 c}{\partial x^2} + \mathcal{O}((\Delta t)^{3/2})\Bigg],\end{aligned} \tag{14}$$

where $R_p(x) \equiv L(x+\Delta_p)/L(x)$ and $R_m(x) \equiv L(x-\Delta_m)/L(x)$.

The usual one-dimensional diffusion equation is

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial c}{\partial x}\right) = D'(x)\frac{\partial c}{\partial x} + D(x)\frac{\partial^2 c}{\partial x^2}, \tag{15}$$

where $D'(x) \equiv \mathrm{d}D(x)/\mathrm{d}x$. This is equivalent to Eq. (14) if the following relations hold:

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\left[R_p(x)T_\ell(x+\Delta_p) + R_m(x)T_\mathrm{r}(x-\Delta_m) - 1\right] = 0, \tag{16}$$

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\left[R_p(x)\Delta_p T_\ell(x+\Delta_p) - R_m(x)\Delta_m T_\mathrm{r}(x-\Delta_m)\right] = D'(x), \tag{17}$$

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\frac{1}{2}\left[R_p(x)\Delta_p^2 T_\ell(x+\Delta_p) + R_m(x)\Delta_m^2 T_\mathrm{r}(x-\Delta_m)\right] = D(x), \tag{18}$$

where $\Delta_p \equiv \Delta_p(x)$ and $\Delta_m \equiv \Delta_m(x)$. Using Eqs. (5) we have the expansions

$$R_p(x) = 1 + L'(x) + \mathcal{O}(\Delta t), \quad R_m(x) = 1 - L'(x) + \mathcal{O}(\Delta t). \tag{19}$$

Substituting these into Eq. (18) and again using Eqs. (5) plus the fact that, from Eq. (2), $L'(x) = \mathcal{O}(\sqrt{\Delta t})$, gives

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} \frac{1}{2} \left[(L(x))^2 (T_\ell(x + \Delta_p) + T_\mathrm{r}(x - \Delta_m)) + \mathcal{O}((\Delta t)^{3/2}) \right] = D(x). \tag{20}$$

In view of Eqs. (2) and (6), plus $T_\ell(x + \Delta_p) = T_\ell(x) + \mathcal{O}(\Delta t)$ and $T_\mathrm{r}(x - \Delta_m) = T_\mathrm{r}(x) + \mathcal{O}(\Delta t)$, this is satisfied exactly. (Alternatively, if we did not assume Eq. (2) then Eq. (20) could be used to establish that $L \approx \sqrt{2D\Delta t}$.) The same procedure applied to Eq. (17) leads to

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t} L(x)[T_\ell(x + \Delta_p) - T_\mathrm{r}(x - \Delta_m)] = -\frac{1}{2} D'(x), \tag{21}$$

which, combined with Eq. (6), gives

$$T_\mathrm{r}(x - \Delta_m) = \frac{1}{2} + \frac{1}{4} L'(x) + \mathcal{O}(\Delta t), \quad T_\ell(x + \Delta_p) = \frac{1}{2} - \frac{1}{4} L'(x) + \mathcal{O}(\Delta t). \tag{22}$$

As noted above, to $\mathcal{O}(\Delta t)$, $T_r(x - \Delta_m)$ and $T_\ell(x + \Delta_p)$ are equal to $T_\mathrm{r}(x)$ and $T_\ell(x)$, respectively. The final relation, Eq. (16), is treated in Appendix A where it is shown to be satisfied exactly.

2.3. Summary of correction terms and extension to higher dimensions

The above calculations show that, in one dimension, a particle at position x at time t should, at time $t + \Delta t$, with probability $T_\mathrm{r}(x)$ move to position $x + \Delta_p(x)$ and with probability $T_\ell(x)$ move to position $x - \Delta_m(x)$, where

$$\Delta_p(x) = L(x) + \frac{1}{2} L(x) L'(x) + \mathcal{O}((\Delta t)^{3/2}), \tag{23}$$

$$\Delta_m(x) = L(x) - \frac{1}{2} L(x) L'(x) + \mathcal{O}((\Delta t)^{3/2}), \tag{24}$$

and

$$T_\mathrm{r}(x) = \frac{1}{2} + \frac{1}{4} L'(x) + \mathcal{O}(\Delta t), \tag{25}$$

$$T_\ell(x) = \frac{1}{2} - \frac{1}{4} L'(x) + \mathcal{O}(\Delta t). \tag{26}$$

Here, $L(x) \equiv \sqrt{2D(x)\Delta t}$ is the uncorrected steplength and $L'(x) \equiv \mathrm{d}L(x)/\mathrm{d}x$.

The extension to higher dimensions is straightforward. Two methods can be used: in the first, in three dimensions, a particle at position (x, y, z) at time t has each of its three coordinates x, y and z updated independently, according to the one-dimensional prescription given above, and the particle is then moved to the new location. In the second method, each timestep Δt is divided into three substeps of duration $\Delta t/3$. In each of these substeps, a direction parallel to the x-, y- or z-axis is chosen at random and the one dimensional algorithm is then used. Numerical tests confirm that, as expected, these two methods give indistinguishable results, so the first method is to be preferred as it is simpler to implement.

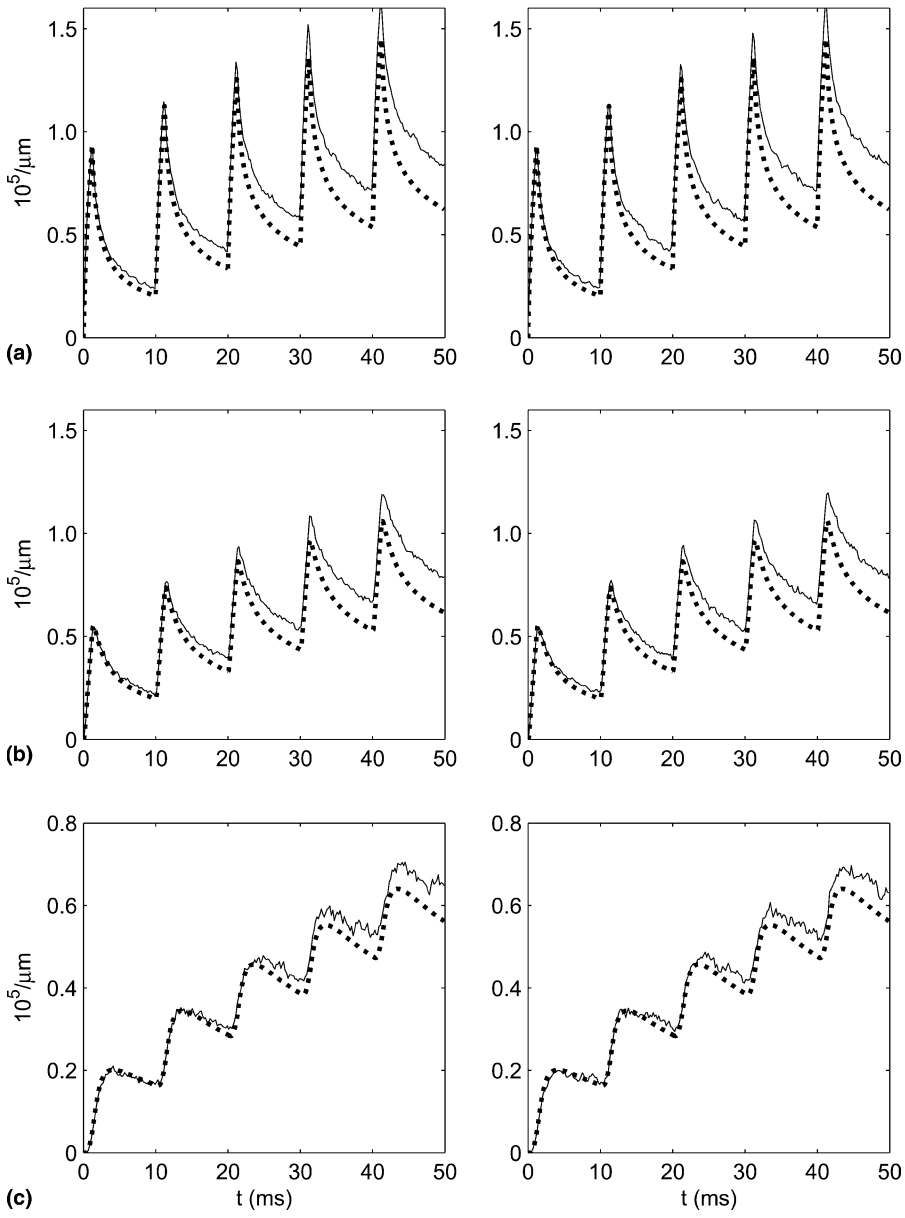

Fig. 2. Comparison of MC and deterministic results for the case of a linearly varying diffusion coefficient, $D(x)$, as given by Eq. (3), with $D_0 = 4\ \mu m^2\ s^{-1}$ and $\alpha = 1.4\ \mu m^{-1}$. A 100 Hz train of action potentials results in the point release of calcium ions, with 7776 ions released over the 1.2 ms following the arrival of each impulse (corresponding to a Ca^{2+} current of 1.08×10^{-20} mol ms^{-1}). These ions diffuse, in one dimension, and the resulting time course of the concentration at distances from the release site of 20, 60 and 180 nm is shown in (a), (b) and (c), respectively. The concentration is expressed as the number of particles per μm, scaled by 10^5. In each panel, the solid line gives the MC result and the broken line the deterministic result obtained by solving the diffusion equation. The resulting concentration, in the MC case, was calculated by averaging the particle count over a 20 nm length and a 200 μs time period. (See [9] for justification of this choice of binning.) In the left column the timestep used was $\Delta t = 1.5$ μs and in the right column it has been reduced to 0.15 μs.

3. Results

As already mentioned, the standard MC method for simulating diffusion with a spatially varying diffusion coefficient cannot be improved by simply reducing the stepsize. This is illustrated in Fig. 2, where the diffusion coefficient $D(x)$ varies linearly with distance according to Eq. (3), and the stepsize $L(x)$ as given by Eq. (2) is used. Calcium ions are released by each action potential in a 100 Hz train, and Ca^{2+} concentration as a function of time is given in panels (a), (b) and (c) for distances from the source of 20, 60 and 180 nm, respectively. The solid lines are the MC results and the broken lines are the deterministic results obtained by numerical solution of the one-dimensional diffusion equation, Eq. (15). It is seen that there is a systematic error that increases with time; reducing the timestep from $\Delta t = 1.5$ μs (left column) to $\Delta t = 0.15$ μs (right column) gives no improvement.

The right column of Fig. 3 shows the corresponding result when the corrections given by Eqs. (23)–(26) are incorporated into the MC scheme; now there is good agreement for all times and distances, and this is achieved with a timestep of $\Delta t = 1.5$ μs. Fig. 4 shows that the corrected method also works well for the more demanding case of the diffusion coefficient of Fig. 1(a); the uncorrected scheme (left column) shows a large error that is completely removed by the correction (right column).

The error resulting from using the uncorrected MC scheme can be even larger for diffusion in three dimensions. The left column of Fig. 5 shows the uncorrected results for the spherically symmetric version of the diffusion coefficient of Fig. 1(a); by a time of 30 ms after the first release and at a distance of 180 μm from the source the MC concentration is more than double the correct value (Fig. 5(c), left panel). Again, the corrected method, implemented as described in Section 2.3, brings the MC results into agreement with the deterministic values (Fig. 5, right column). As a final test, the method was applied to a three-dimensional case that was not spherically symmetric (Fig. 6) and again use of the correction terms produced good agreement.

4. Discussion

A 'standard' method of improving the accuracy of a numerical procedure is to reduce a timestep or a stepsize. However, this does not work in the present case: reducing the timestep (and hence the stepsize) does not lead to any improvement in accuracy. The reason for this was clear from our previous work on the Gaussian-step correction [9], where it was explicitly shown that the leading correction per step is proportional to Δt and since the number of steps is proportional to $1/\Delta t$ the total error is almost independent of Δt.

A notable aspect of the present calculation is that both the steplength and the transition probability are modified and it is interesting to note that the correction to both involves the same multiplicative factor, as is apparent when Eqs. (23) and (25) are written as $\Delta_p(x) = L(x)[1 + \frac{1}{2}L'(x) + \mathcal{O}(\Delta t)]$ and $T_r(x) = \frac{1}{2}[1 + \frac{1}{2}L'(x) + \mathcal{O}(\Delta t)]$, respectively. It was not immediately apparent to us that altering both the step length and the transition probability was the way to proceed, and early attempts to correct the MC scheme by altering one or the other were not successful. We cannot establish rigorously that both modifications must be made, but we offer the following observations in support of such a necessity.

For the case of diffusion in one dimension under a constant diffusion coefficient D_0, the probability distribution for finding a particle at location x at time t, given that it was released from the origin at time $t = 0$, is given by the Gaussian distribution

$$f_X(x) = \frac{1}{\sqrt{4\pi D_0 t}} e^{-x^2/4D_0 t}. \tag{27}$$

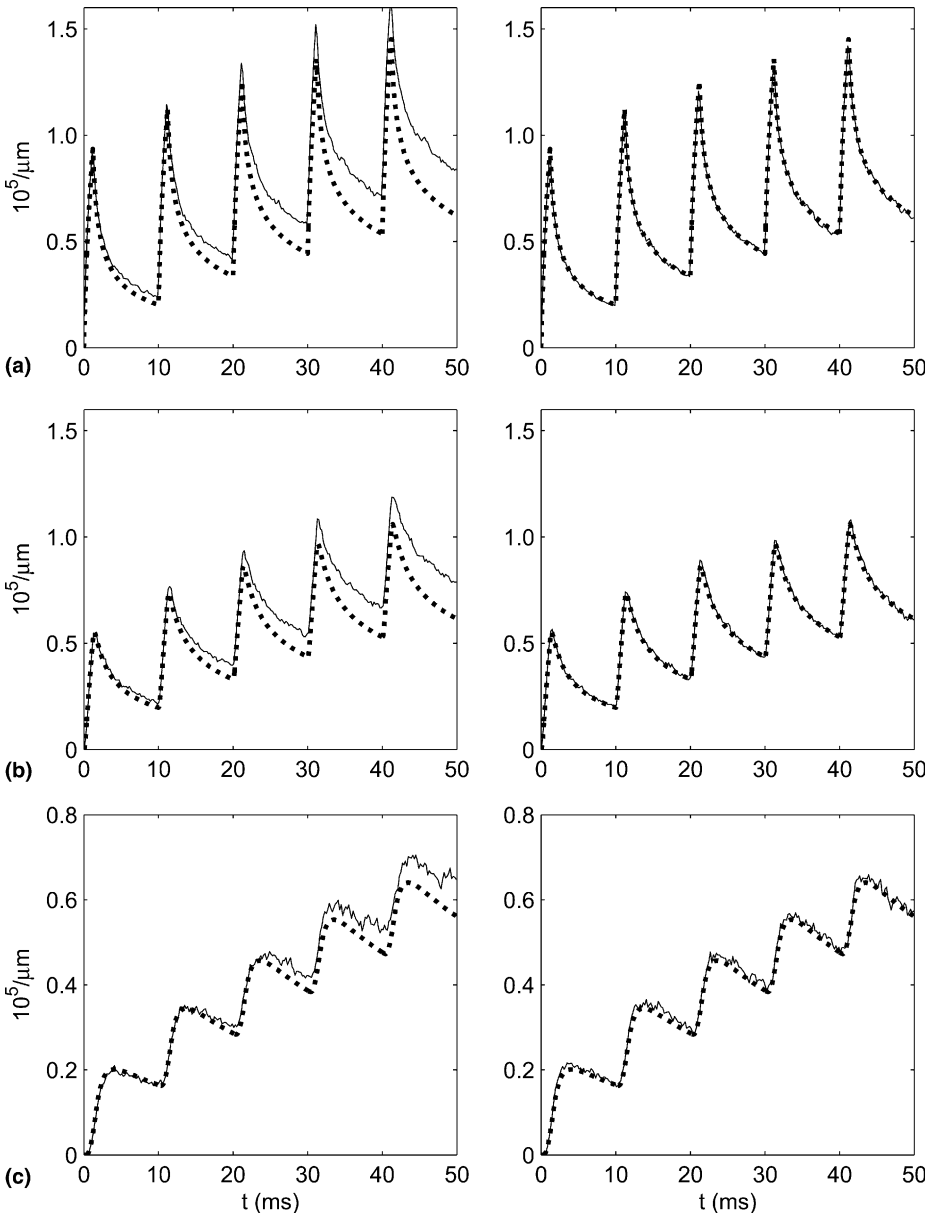

Fig. 3. Ca^{2+} diffusion under a linearly varying diffusion coefficient. The Ca^{2+} release protocol is the same as for Fig. 2; the diffusion coefficient is given by Eq. (3) with $D_0 = 4\ \mu m^2\ s^{-1}$ and $\alpha = 1.4\ \mu m^{-1}$. The left column shows the MC simulation results (solid lines) when the uncorrected steplength $L(x)$ is used, compared with the solution of the diffusion equation (broken lines) (and is the same as the left column of Fig. 2). The right column shows the corresponding results when the MC scheme is corrected using Eqs. (23)–(26). In both MC calculations the timestep used was $\Delta t = 1.5\ \mu s$.

This is, of course, a symmetric distribution with maximum at $x = 0$. The effect of a spatially varying diffusion coefficient $D(x)$ is to skew the distribution and also move the peak from $x = 0$. For example, for the linearly varying diffusion coefficient given by Eq. (3) the distribution is [9]

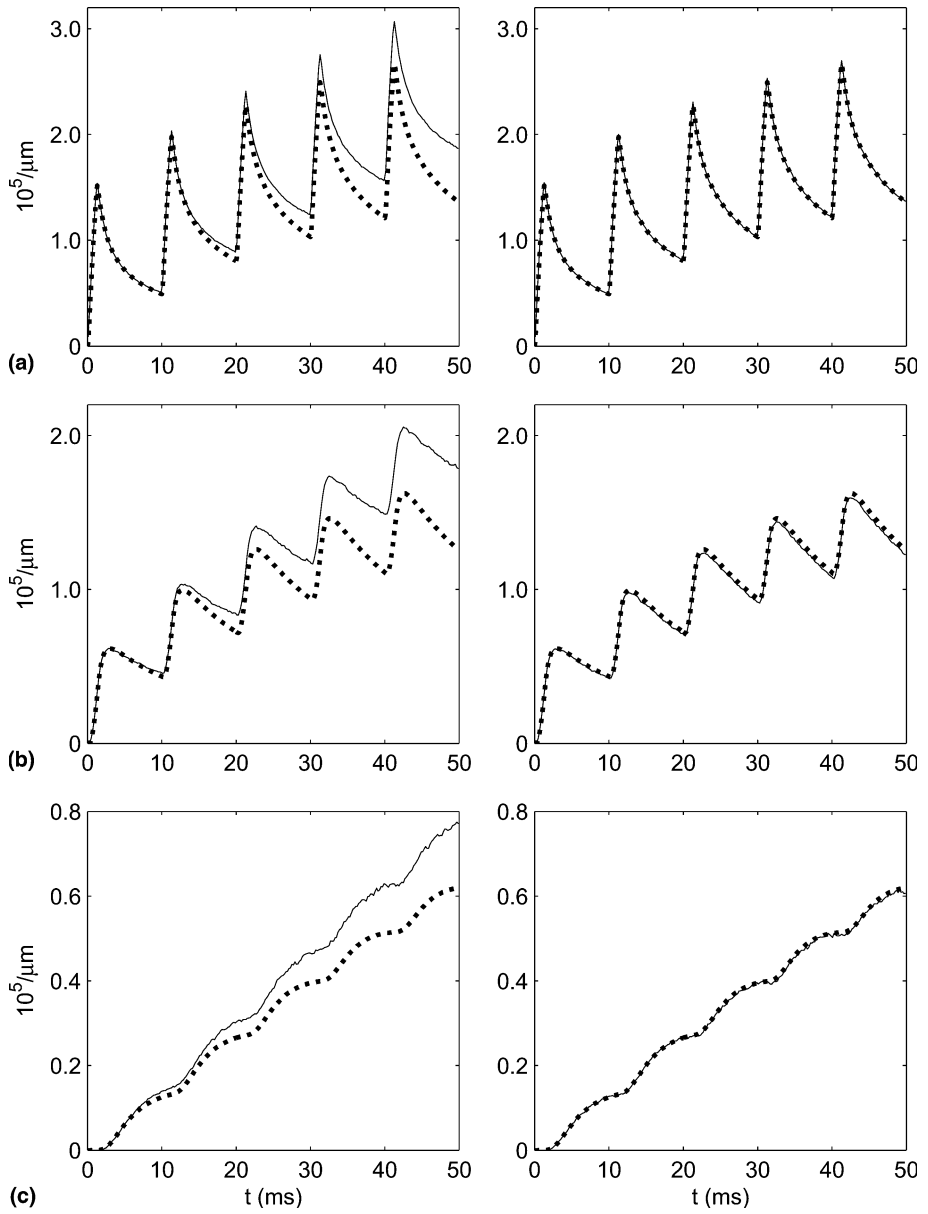

Fig. 4. Comparison of MC and deterministic results for the case of a variable diffusion coefficient, $D(x)$, as given in Fig. 1(a), with the left column using the uncorrected MC scheme and the right column using the corrections of Eqs. (23)–(26). The remaining details are as for Fig. 1, except that in order to improve comparison between MC and deterministic results the number of particles released per impulse has been increased by a factor of 10 (to 77,760) and the timestep has been reduced to $\Delta t = 0.15$ μs.

$$f_X(x) = \frac{1}{D_0|\alpha|t} \mathrm{e}^{-(2+\alpha x)/D_0\alpha^2 t} I_0\left(\frac{2\sqrt{1+\alpha x}}{D_0\alpha^2 t}\right), \tag{28}$$

where $I_0(\cdot)$ is a modified Bessel function. This is a skewed distribution, with peak at $x \approx -\alpha D_0 t/2$.

Thus corrections to the constant-step MC scheme must lead to a skewed distribution with peak displaced from $x = 0$. This cannot be achieved with a transition probability of 1/2 if the random walk takes place on a

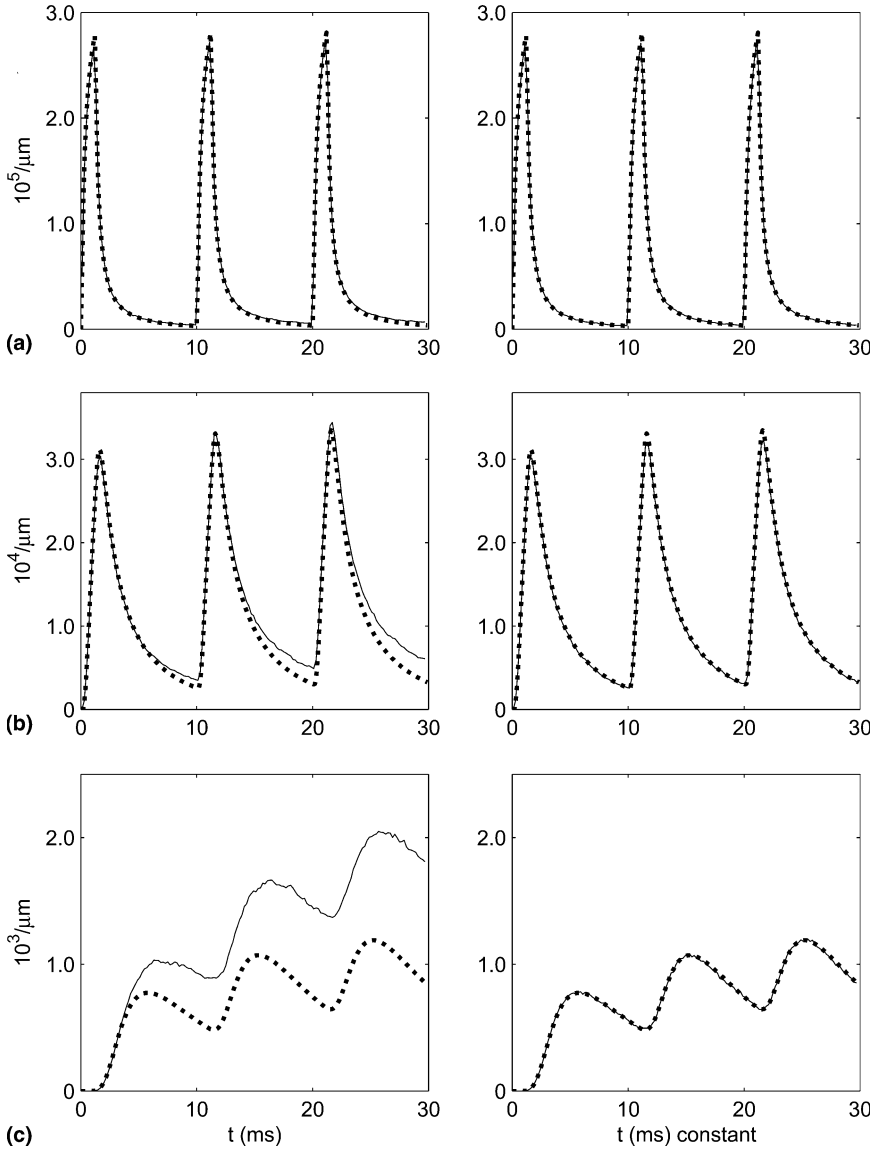

Fig. 5. Comparison of MC and deterministic results for diffusion in three dimensions with a spherically symmetric variable diffusion coefficient. The diffusion coefficient is that of Fig. 1(a), with x replaced by the radial coordinate r. The concentration in the MC case was calculated by averaging the particle count over a spherical shell of thickness 10 nm and a 200 μs time interval and the number of particles released per impulse was 62,208. The remaining details are as for Fig. 4, with panels (a), (b) and (c) now giving the concentration time courses at radial distances of 20, 60 and 180 nm, respectively, from the source. Note that a different scale has been used on the vertical axes in (a), (b) and (c).

fixed lattice such as that given by Eq. (1), since as far as the lattice points are concerned there is complete left–right symmetry in the walk and so the distribution will still have its maximum at $x = 0$, though it will be skewed. If one drops the requirement of a fixed lattice, then it may be possible to find a correction using steplength only, but we have not found any systematic way of doing this. The other extreme is to set $\Delta_p = \Delta_m = L(x)$ and try to find corrections to the transition probability. This would displace the peak of

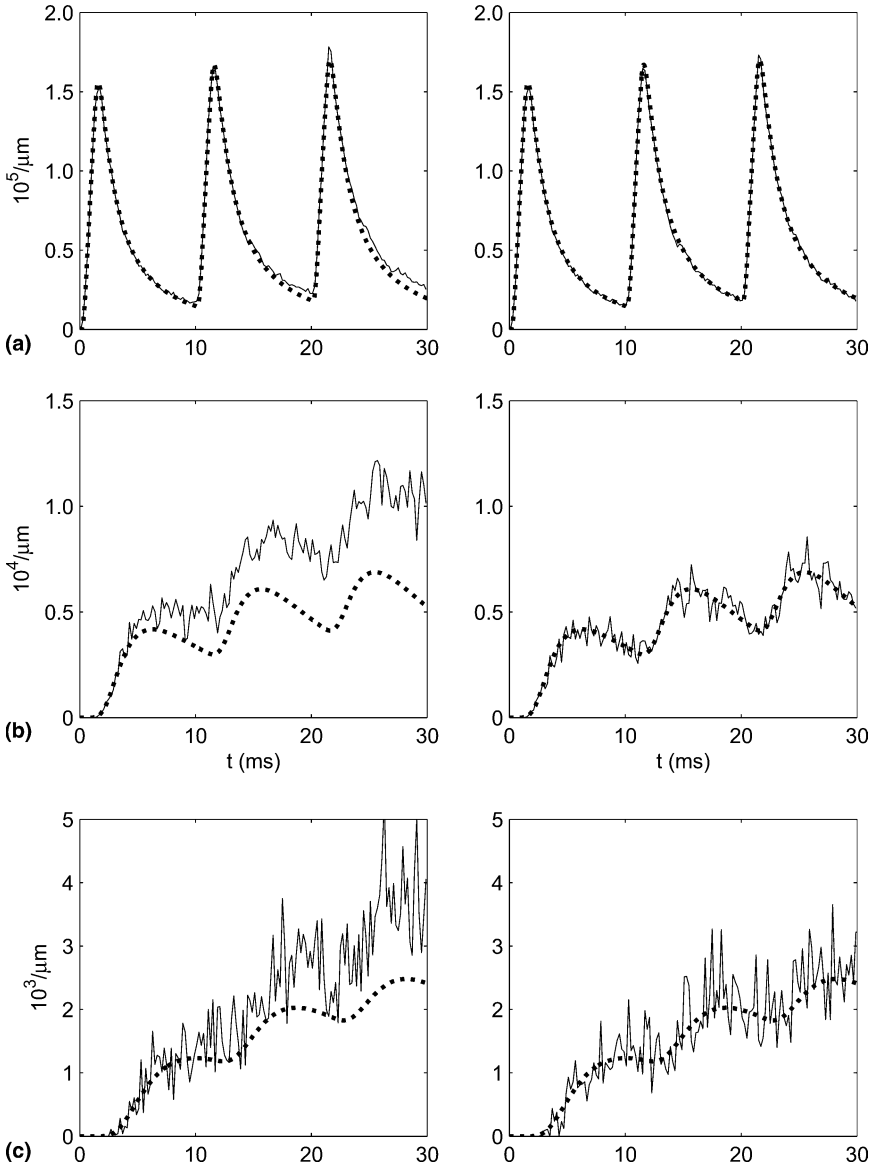

Fig. 6. Comparison of MC and deterministic results for diffusion in three dimensions with a non-spherically symmetric variable diffusion coefficient. The diffusion coefficient is $D(x,y,z) = \widehat{D}(1 - 0.8u(|x|)u(|y|)u(z))$, where the function $u(x)$ is given in Fig. 1(a). The parameter values are again $\widehat{D} = 4\ \mu m^2\ s^{-1}$, $A = 35\ \mu m^{-1}$ and $b = 0.2\ \mu m$, except that in $u(z)$, A has the value $50\ \mu m^{-1}$. The diffusion takes place in the half space $z > 0$, 311,040 particles are released from the origin at each impulse, and a timestep $\Delta t = 0.15\ \mu s$ is used. The MC concentrations were calculated using a cubical box of side 10 nm centred on the points $(x,y,z) = (0,0,60\ nm)$, $(0,0,180\ nm)$ and $(180,180,20\ nm)$, in panels (a), (b) and (c), respectively. The deterministic results are for the same points. Note that a different scale has been used on the vertical axes in (a), (b) and (c).

the distribution from the origin, but numerical experiments indicate that for any reasonable sort of correction terms the distribution remains close to Gaussian. Thus while it is again conceivable that such corrections could be found, we have not been able to develop any systematic approach along these lines.

To summarize, in this paper, we have derived simple formulas, Eqs. (23)–(26), for correcting the standard fixed-step MC method in the case where the diffusion coefficient varies with distance. These are given explicitly for one dimension, but are immediately applicable to higher dimensions, as described in Section 2.3. The calculations presented here all refer to a particular neurobiological context, but the method is quite general and applicable to any problem involving nonhomogeneous diffusion.

Acknowledgement

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Appendix A. Investigation of Eq. (16)

To establish the validity of Eq. (16), we need to calculate terms to higher order than has been done in the body of the text. The extensions to Eqs. (5) are

$$\Delta_p = L + \frac{1}{2}LL' + \frac{1}{4}(LL'^2 + L^2L'') + \mathcal{O}((\Delta t)^2), \tag{29}$$

$$\Delta_m = L - \frac{1}{2}LL' + \frac{1}{4}(LL'^2 + L^2L'') + \mathcal{O}((\Delta t)^2), \tag{30}$$

where all quantities are to be evaluated at x. These lead to the extensions to Eqs. (19):

$$R_p = 1 + L' + \frac{1}{2}(L'^2 + LL'') + \mathcal{O}((\Delta t)^{3/2}), \tag{31}$$

$$R_m = 1 - L' + \frac{1}{2}(L'^2 + LL'') + \mathcal{O}((\Delta t)^{3/2}), \tag{32}$$

where again all quantities are to be evaluated at x. Now, $T_\ell(x+\Delta_p) = T_\ell(x) + \Delta_p T'_\ell(x) + \mathcal{O}((\Delta t)^{3/2}) = T_\ell(x) - \frac{1}{4}LL'' + \mathcal{O}((\Delta t)^{3/2})$. Similarly, $T_\mathrm{r}(x-\Delta_m) = T_\mathrm{r}(x) - \frac{1}{4}LL'' + \mathcal{O}((\Delta t)^{3/2})$, so

$$T_\ell(x+\Delta_p) + T_\mathrm{r}(x-\Delta_m) = 1 - \frac{1}{2}LL'' + \mathcal{O}((\Delta t)^{3/2}). \tag{33}$$

Also, from Eq. (22),

$$T_\ell(x+\Delta_p) - T_\mathrm{r}(x-\Delta_m) = -\frac{1}{2}L' + \mathcal{O}(\Delta t). \tag{34}$$

Using Eqs. (31)–(34) gives

$$R_p(x)T_\ell(x+\Delta_p) + R_m(x)T_\mathrm{r}(x-\Delta_m) - 1 = \mathcal{O}((\Delta t)^{3/2}), \tag{35}$$

so Eq. (16) is satisfied exactly.

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