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Abstract

We construct in this paper a Monte Carlo method in order to approach solutions of multi-dimensional Stochastic Differential Equations processes which relies on the importance sampling technique. Our method is based on the random walk on squares/rectangles method and the main interest of this construction is that the weights are easily computed from the density of the one-dimensional Brownian motion. The advantage we take on the Euler scheme is that this method allows us to get a better simulation of diffusions when one has really to take care of the boundary conditions. Moreover, it provides a good alternative to perform variance reduction techniques and simulation of rare events.

Keywords: Stochastic Differential Equations, Monte Carlo methods, Random walk on squares, Random walk on rectangles, variance reduction, simulation of rare events, Dirichlet/Neumann problems

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1 Introduction

Monte Carlo methods are sometimes a useful, if not the only way, to solve numerically PDE involving an operator of the form

$$L = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(.)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i(.)\frac{\partial}{\partial x_i}.$$

As L is the infinitesimal generator associated to the solution of the stochastic differential equation (SDE)

$$X_t = X_0 + \int_0^t \sigma(X_s)\,\mathrm{d}B_s + \int_0^t b(X_s)\,\mathrm{d}s \text{ with } \sigma\sigma^* = a, \tag{1}$$

the solution, on the cylinder $[0,T]\times D$, of the parabolic PDE

$$\begin{cases} \dfrac{\partial u(t,x)}{\partial t} + Lu(t,x) = 0, \\ u(T,x) = g(x) \text{ on } x \in D, \\ u(t,x) = \phi(t,x) \text{ on } (t,x) \in [0,T]\times \partial D \end{cases}$$

is given by

$$u(t,x) = \mathbb{E}_{t,x}[g(X_T); T \le \tau] + \mathbb{E}_{t,x}[\phi(\tau, X_\tau); \tau < T],$$

where τ stands for the first exit time of X from the domain D, when X started from x at time t. Thus, an approximation of $u(t,x)$ can be obtained by averaging $g(X_T)\mathbb{1}_{T\le\tau}$ and $\phi(\tau, X_\tau)\mathbb{1}_{\tau<T}$ over a large number of realizations of paths of X. Elliptic PDE or additional terms may be considered as well.

Up to now, many methods have been proposed to simulate X. For a large spectra of these methods, see for example the books of P. Kloeden and E. Platen [KP92] and of G.N. Milstein and M.V. Tretyakov [MT04]. Most of these methods are extensions of the Euler scheme, which provides a very efficient way to simulate (1) in the whole space. This method becomes harder to set up in a bounded domain, either with an absorbing or a reflecting boundary condition. Nevertheless some refinements have been proposed (see for example [Pet95, Gob00, Sło01, Gob01, JL03, BGT04]). To improve the quality of the simulation or fasten it, various variance reduction techniques can be considered; see for example [New94, HP02, KHP02, ZS04, Aro04a, Aro04b, Bar05, Keb05], this list being far from being exhaustive.

In the simplest situation, for $a = \mathrm{Id}$ and $b = 0$, the diffusion process to deal with is the Brownian motion, and E. Muller proposed in 1956 a

very simple scheme to solve a Dirichlet boundary value problem, called the *random walk on spheres* [Mul56]. The idea is to simulate successively, for the Brownian motion, the first exit position from the largest sphere included in the domain and centered in the starting point. This procedure is iterated until the exit point is close enough to the boundary. Nevertheless, simulating the exit time from a sphere is numerically costly. In [MR93], G.N. Milstein and N.F. Rybkina proposed to use this scheme for solving (1) by freezing locally the value of the coefficients. In a first approach, spheres (that become ellipsoids) were used, and then in [Mil95] (see also their book [MT04]), G.N. Milstein and M.V. Tretyakov used time-space parallelepipeds with a cubic space basis. In this last approach, it is easier to keep track of the time but the involved random variables are costly to simulate. Of course, one may use tabulated values, but this becomes memory consuming as the random variables to simulate depend on one or two parameters. Nevertheless, for the Brownian motion, this method is a good alternative to the random walk on spheres: see [CL02] for an application in a geophysical problem.

In [DL06], we have proposed a scheme for simulating the exact exit time and position from a rectangle for the Brownian motion starting at any point inside it. This method have the following advantage over the random walk on spheres method: it can be used whatever the dimension and, as for the random walk on squares, a constant drift term may be added. In addition, the rectangles may be chosen prior to any simulation, and not dynamically. Besides, there is no need to consider smaller and smaller spheres or squares when the particle approaches the boundary. Finally, the method is also easily modified in order to simulate diffusion processes conditioned not to reach a part of the boundary for example. However, this method can be too costly for simulating SDEs, because it takes too much time if the "steps" are too small.

The method we propose here is based on the idea to simulate the first exit time and position from a parallelepiped by using an importance sampling technique (see for example [Fis96, Gla04]). The exit time and position from a parallelepiped for a Brownian motion with locally frozen coefficients is chosen arbitrarily, and a weight is computed at each simulation. By repeating this procedure, we get the density on the boundary or at a given time of the particles, by weighting their trajectories. As we explain it later on, the weights are rather easily deduced from the density of the one-dimensional Brownian motion killed when it exits from $[-1, 1]$, and all involved expressions are numerically easy to implement.

In fact, this algorithm is slower than the Euler scheme for smooth situations, but it is faster than the random walk on squares [MT04, CL02] and the random walk on rectangles [DL06]. It can be used to simulate the Brownian

motion as well as solutions of stochastic differential equations for specific complex situations as: (a) complex geometries (the boundary conditions are correctly taken into account); (b) fast estimation of the exit time of a domain for the Brownian motion (only few rectangles are needed); (c) variance reduction; (d) simulation of rare events.

This algorithm could be relevant for many domains: finance, physics, biology, geophysics, etc. It may also be used locally (for example, it can be mixed with the Euler scheme and used when the particle is close to the boundary) or combined with other algorithms, such as the one proposed in [CDMLL06] for simulating rare events.

We end this article with few numerical simulations illustrating various examples. It has to be noted that choosing "good" distributions for the exit time and position from a rectangle is not an easy task in order to reduce the variance. We then plan to study in the future how to construct some algorithms to minimize the variance, as in [Aro04a, Bar05], which appears to be a high dimension optimization problem.

Outline. In Section 2, we present the importance sampling technique applied to the exit time and position for a (drifted) Brownian motion from a rectangle. In Section 3, we recall briefly some results about the density of the one-dimensional Brownian motions with different boundary conditions, whose expressions are given in Appendix A. In Section 4, we present our algorithm and compute its weak error. Four test cases are presented in Section 5, where we compare also our algorithm with other methods.

2 Exit time and position from a right parallelepiped

In this section, we show how to simulate the exit time and position from a right time-space parallelepiped, that is the set obtained by the set products of intervals in each direction of the space and the time.

For $L_1, \ldots, L_d > 0$, let R be the right parallelepiped $[-L_1, L_1] \times \cdots \times [-L_d, L_d]$.

We fix $T > 0$, with possibly $T = +\infty$. The sides of the parallelepiped

$R_T = [0,T] \times R$ are denoted by

$$\begin{aligned}
S_{i,\eta} &= [0,T] \times [-L_1, L_1] \times \cdots \times [-L_{i-1}, L_{i-1}] \times \{\eta L_i\} \\
&\qquad \times [-L_{i+1}, L_{i+1}] \times \cdots \times [-L_d, L_d] \text{ for } (i,\eta) \in [\![1,d]\!] \times \{-1,1\}, \\
S_{0,1} &= \{T\} \times [-L_1, L_1] \times \cdots \times [-L_d, L_d] \text{ if } T < +\infty, \\
S_{0,-1} &= \{0\} \times [-L_1, L_1] \times \cdots \times [-L_d, L_d].
\end{aligned}$$

In other words, each side of R is labelled by a couple $(i,\eta) \in [\![1,d]\!] \times \{-1,1\}$ with the convention that the side is perpendicular to the unit vector in the i-th direction: See Figure 1.

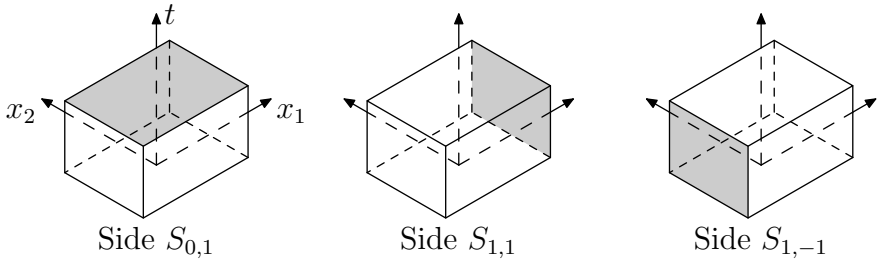

Figure 1: Convention for the sides of $R_T = [0,T] \times R$.

We are interested in a diffusion process living in R_T. Neumann boundary conditions hold possibly on some of the lateral sides of $[0,T] \times R$. The set $\mathfrak{R}$ will be the subset of $[\![1,d]\!] \times \{-1,1\}$ on which the diffusion is reflected (possibly, $\mathfrak{R} = \emptyset$). If $T < +\infty$, we set $\mathfrak{S} = \{(0,1)\} \cup [\![1,d]\!] \times \{-1,1\}$ the set of all sides, except $S_{0,-1}$ (that corresponds to $\{0\} \times R$). If $T = +\infty$, we set $\mathfrak{S} = [\![1,d]\!] \times \{-1,1\}$. Finally, we denote by $\mathfrak{A} = \mathfrak{S} \setminus \mathfrak{R}$ the set of sides on which the diffusion is killed.

Let $B = (B^1, \ldots, B^d)$ be a d-dimensional Brownian motion and $\mu = (\mu^1, \ldots, \mu^d)$ a vector of $\mathbb{R}^d$. For $i = 1, \ldots, d$, we set

$$\gamma_{(i,\eta)} = \begin{cases} -\eta & \text{if } (i,\eta) \in \mathfrak{R} \text{ (reflection)}, \\ 0 & \text{if } (i,\eta) \in \mathfrak{A} \text{ (absorption)}. \end{cases}$$

We consider now the d-dimensional diffusion process X whose coordinates are, for $x = (x_1, \ldots, x_d) \in R$,

$$X_t^i = x_i + B_t^i + \mu_i t + \gamma_{(i,1)} \ell_t^{L_i}(X^i) + \gamma_{(i,-1)} \ell_t^{-L_i}(X^i) \tag{2}$$

where $\gamma_{(i,-1)} \in \{0,1\}$, $\gamma_{(i,1)} \in \{-1,0\}$, $\ell_t^{\pm L_i}(X^i)$ is the symmetric local time of X^i at $\pm L_i$. If $\gamma_{(i,1)} = -1$ (resp. $\gamma_{(i,-1)} = 1$), then the i-th coordinate X^i

is reflected at L_i (resp. $-L_i$). If $\gamma_{(i,\pm 1)} = 0$, then the i-th coordinate of X^i is killed at $\mp L_i$.

We denote by $\mathbb{P}_x$ the distribution of X starting at $X_0 = x$.

We define $\tau_0 = T$, $\tau_i = \inf\{t > 0 \,|\, |X_t^i| > L_i\}$ for $i = 1, \ldots, d$ and $\tau = \min_{i=0,\ldots,d} \tau_i$. In addition, we set $J = \operatorname{argmin}_{i=0,\ldots,d} \tau_i$ which means that the J-th component of X is the first to exit if $J \neq 0$. If $J \geq 1$, we set $\varepsilon = X_{\tau_J}^J / L_J \in \{-1, 1\}$. If $J = 0$, then we set $\varepsilon = 1$ and this means that X has not reached the sides of $\mathfrak{R}$ before T. The couple (J, ε) labels the side in $\mathfrak{A}$ of the parallelepiped $R_T = [0, T] \times R$ which is reached first by the diffusion X. Note that with our convention, the sides on which the process is reflected cannot be reached, so that $\tau_i = +\infty$ if X^i is reflected both at $-L_i$ and L_i.

We are interested in computing $\mathbb{E}_x[f(\tau, X_\tau)]$ by a Monte Carlo method for a bounded, measurable function f. Instead of simulating (τ, X_τ) we simulate some random variables according to the following procedure:

Algorithm 1. Let x be a point of R.

(1) Choose a side $S_{J,\varepsilon}$ with $(J, \varepsilon) \in \mathfrak{A}$ drawn according to an arbitrary set of discrete probabilities $\{\alpha_{i,\eta}\}_{(i,\eta)\in\mathfrak{A}}$ with $\alpha_{i,\eta} > 0$ for $(i, \eta) \in \mathfrak{A}$ and $\sum_{(i,\eta)\in\mathfrak{A}} \alpha_{(i,\eta)} = 1$.

(2) Choose an exit time and position (Θ, Z) according to an arbitrary density $k_{J,\varepsilon}$ on $S_{J,\varepsilon}$.

(3) Finally, compute the value of the random variable $M_{J,\varepsilon}(\Theta, Z)$ — called a *weight* — which is defined such that

$$\mathbb{E}_x[f(\tau, X_\tau)] = \widehat{\mathbb{E}}_x[M_{J,\varepsilon}(\Theta, Z) f(\Theta, Z)]$$

where $\widehat{\mathbb{P}}_x$ is the distribution of $(J, \varepsilon, \Theta, Z)$.

If $\{(J^{(i)}, \varepsilon^{(i)}, \Theta^{(i)}, Z^{(i)}, w^{(i)})\}_{i=1,\ldots,N}$ are N independent realizations of the random variables $(J, \varepsilon, \Theta, Z, M_{J,\varepsilon}(\Theta, Z))$ constructed as above, the law of large numbers ensures that

$$\mathbb{E}_x[f(\tau, X_\tau)] = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} w^{(i)} f(\Theta^{(i)}, Z^{(i)}).$$

Here, we have simply followed the importance sampling technique. The main feature of our approach is that the weights can be evaluated rather easily.

Proposition 1. *For $(i, \eta) \in \mathfrak{A}$, $i \neq 0$, $\theta > 0$ and $z \in S_{i,\eta}$,*

$$M_{i,\eta}(\theta, z) = \frac{\mathbb{P}_{x_i}[\tau_i = \theta, X_\theta^i = \eta L_i]}{\alpha_{i,\eta} k_{i,\eta}(\theta, z)} \prod_{\substack{j=1,\ldots,d \\ j\neq i}} \mathbb{P}_{x_j}[X_\theta^j = z_j, \tau_j > \theta]. \tag{3}$$

If $T < +\infty$,

$$M_{0,1}(T,z) = \frac{1}{\alpha_{0,1} k_{0,1}(T,z)} \prod_{j=1,\dots,d} \mathbb{P}_{x_j}[X_T^j = z_j, \tau_j > T]. \tag{4}$$

Remark 1. In order to evaluate $M_{i,\eta}$ with (3) and (4), there is no need to know $\mathbb{P}_x[(J,\varepsilon) = (i,\eta)]$. Thus $M_{i,\eta}$ depends only on the one-dimensional distributions of the drifted Brownian motion.

Proof. We now define a probability measure $\mathbb{P}'_x$ such that for $(i,\eta) \in \mathfrak{A}$,

$$\mathbb{P}'_x[\cdot \,|\, (J,\varepsilon) = (i,\eta)] = \mathbb{P}_x[\cdot \,|\, (J,\varepsilon) = (i,\eta)] \text{ and } \mathbb{P}'_x[(J,\varepsilon) = (i,\eta)] = \alpha_{i,\eta}.$$

For $(i,\eta) \in \mathfrak{A}$, we define a probability density $k_{i,\eta} > 0$ on $S_{i,\eta}$. We then define a new probability $\widehat{\mathbb{P}}_x$ such that $k_{i,\eta}$ is the density of (τ, X_τ) under $\mathbb{P}'_x[\cdot \,|\, (J,\varepsilon) = (i,\eta)]$ (or equivalently, $\mathbb{P}_x[\cdot \,|\, (J,\varepsilon) = (i,\eta)]$ as the two probabilities $\mathbb{P}_x$ and $\mathbb{P}'_x$ are equal when conditioned to $\{(J,\varepsilon) = (i,\eta)\}$).

Let f be a measurable, bounded function on ∂R_T. We are interested in evaluating $\mathbb{E}_x[f(\tau, X_\tau)]$ and we are looking for a *weight* $M_{i,\eta}$ such that

$$\mathbb{E}_x[f(\tau, X_\tau)] = \widehat{\mathbb{E}}_x[M_{J,\varepsilon}(\Theta, Z) f(\Theta, Z)],$$

where (J,ε) is drawn according to the probabilities $\widehat{\mathbb{P}}_x[(J,\varepsilon) = (i,\eta)] = \alpha_{i,\eta}$ for $(i,\eta) \in \mathfrak{A}$ and (Θ, Z) is drawn according to the density $k_{i,\eta}$.

We remark first that if $p_{i,\eta} = \mathbb{P}_x[(J,\varepsilon) = (i,\eta)]$ for (i,η) in $\mathfrak{A}$, then

$$\mathbb{E}_x[f(\tau, X_\tau)] = \mathbb{E}'_x[f(\tau, X_\tau) p_{J,\varepsilon} / \alpha_{J,\varepsilon}].$$

Secondly, for $(i,\eta) \in \mathfrak{A}$,

$$\begin{aligned}
&\mathbb{E}'_x[f(\tau, X_\tau) \,|\, (J,\varepsilon) = (i,\eta)] \\
&\quad = \int_{S_{i,\eta}} f(\theta, z) \mathbb{P}_x[\tau_i = \theta, X_\theta = z \,|\, (J,\varepsilon) = (i,\eta)] \,\mathrm{d}\theta \,\mathrm{d}z_1 \cdots \mathrm{d}z_d \\
&\qquad\qquad = \widehat{\mathbb{E}}_x \left[f(\Theta, Z) M'_{i,\eta}(\Theta, Z) \big| (J,\varepsilon) = (i,\eta) \right],
\end{aligned}$$

where (Θ, Z) is a realization of a random variable with density $k_{i,\eta}$ and

$$M'_{i,\eta}(\Theta, Z) = \frac{\mathbb{P}_x[\tau_i = \Theta, X_\Theta = Z \,|\, (J,\varepsilon) = (i,\eta)]}{k_{i,\eta}(\Theta, Z)}.$$

Hence,

$$\mathbb{E}_x[f(\tau, X_\tau)] = \widehat{\mathbb{E}}_x[f(\Theta, Z) M_{J,\varepsilon}(\Theta, Z)]$$

with $M_{J,\varepsilon}(\theta,z) = M'_{J,\varepsilon}(\theta,z)p_{J,\varepsilon}/\alpha_{J,\varepsilon}$.

It remains now to remark that for $(i,\eta) \in \mathfrak{A}$ and $i \neq 0$,

$$\begin{aligned} M_{i,\eta}(\theta,z) &= \frac{1}{\alpha_{i,\eta}k_{i,\eta}(\theta,z)}\mathbb{P}_x[\tau_i = \theta, X_\theta = z, (J,\varepsilon) = (i,\eta)] \\ &= \frac{1}{\alpha_{i,\eta}k_{i,\eta}(\theta,z)}\mathbb{P}_x[\tau_i = \theta, X^i_\theta = \eta L_i, X^j_\theta = z_j, \tau^j > \theta \text{ for } j \neq i]. \end{aligned}$$

The independence of the coordinates leads to (3). If $T < +\infty$, then we also define

$$M_{0,1}(T,z) = \frac{1}{\alpha_{0,1}k_{0,1}(T,z)}\mathbb{P}_x\left[X_T = z, \min_{i=1,\dots,d}\tau^i > T\right]$$

which leads to (4). □

We can now turn to compute these probabilities: For $i = 1,\dots,d$, let $p^i(t,x,y)$ be the solution of

$$\begin{cases} \dfrac{\partial p^i(t,x,y)}{\partial t} = \dfrac{1}{2}\dfrac{\partial^2 p^i(t,x,y)}{\partial y^2} + \mu_i \dfrac{\partial p^i(t,x,y)}{\partial y}, \text{ for } (t,x,y) \in \mathbb{R}_+ \times (-L_i,L_i)^2, \\ p^i(t,x,y) \xrightarrow[t\searrow 0]{} \delta_x(y) \text{ for } (x,y) \in (-L_i,L_i)^2, \end{cases} \tag{5}$$

with the following boundary conditions

$$\begin{aligned} p^i(t,x,-L_i) &= 0 \text{ (Dirichlet b.c.) if } (i,-1) \in \mathfrak{A}, \\ \frac{\partial p^i(t,x,-L_i)}{\partial y} &= 0 \text{ (Neumann b.c.) if } (i,-1) \in \mathfrak{R}, \\ p^i(t,x,L_i) &= 0 \text{ (Dirichlet b.c.) if } (i,1) \in \mathfrak{A}, \\ \frac{\partial p^i(t,x,L_i)}{\partial y} &= 0 \text{ (Neumann b.c.) if } (i,1) \in \mathfrak{R}. \end{aligned}$$

Thus, p^i denotes the density of the drifted Brownian motion X^i with possibly some reflection at the endpoints of $(-L_i,L_i)$, and killed when it exits from this interval by an endpoint where no reflection holds. If f is a bounded, measurable function from $[-L_i,L_i]$ to $\mathbb{R}$, then

$$\mathbb{E}_x[f(X^i_t); t < \tau] = \int_{-L_i}^{L_i} p^i(t,x,y)f(y)\,\mathrm{d}y.$$

We introduce the *scale function* $\Phi^{i,+}$ of X^i defined by,

$$\text{for } y \in [-L_i,L_i],\ \Phi^{i,+}(y) = \begin{cases} \dfrac{e^{2\mu_i L_i} - e^{-2\mu_i y}}{e^{2\mu_i L_i} - e^{-2\mu_i L_i}} \text{ if } \mu_i \neq 0, \\ \dfrac{y + L_i}{2L_i} \text{ if } \mu_i = 0. \end{cases}$$

The function $\Phi^{i,+}(y)$ has been normalized so that $\Phi^{i,+}(L_i) = 1$. Let us note that $\Phi^{i,+}(x_i) = \mathbb{P}_{x_i}[X^i_{\tau_i} = L_i]$ if Dirichlet boundary conditions hold at both points $-L_i$ and L_i. We also set $\Phi^{i,-}(y) = 1 - \Phi^{i,+}(y)$.

If Dirichlet boundary conditions hold at both $-L_i$ and L_i, then we set for $t > 0$ and $(x, y) \in [-L_i, L_i]^2$,

$$p^{i,\pm}(t, x, y) = p^i(t, x, y)\frac{\Phi^{i,\pm}(y)}{\Phi^{i,\pm}(x)}.$$

Via a Doob transform, we obtain for a function f bounded and measurable

$$\mathbb{E}_x[f(X^i_t); t < \tau \,|\, X^i_{\tau_i} = \pm L_i] = \int_{-L_i}^{L_i} p^{i,\pm}(t, x, y) f(y)\,\mathrm{d}y.$$

We may now set for $x \in (-L_i, L_i)$,

$$q^i(t, x) = -\int_{-L_i}^{L_i} \frac{\partial p^i}{\partial t}(t, x, y) f(y)\,\mathrm{d}y \tag{6}$$

$$\text{and } q^{i,\pm}(t, x) = -\int_{-L_i}^{L_i} \frac{\partial p^{i,\pm}}{\partial t}(t, x, y) f(y)\,\mathrm{d}y. \tag{7}$$

We can easily deduce that

$$\int_0^t q^i(s, x)\,\mathrm{d}s = \mathbb{P}_x[\tau_i \le t] \text{ and } \int_0^t q^{i,\pm}(s, x)\,\mathrm{d}s = \mathbb{P}_x[\tau_i \le t \,|\, X^i_{\tau_i} = \pm L_i].$$

In other words, $q^i(t, x)$ (resp. $q^{i,\pm}(t, x)$) is the density of the first exit time from $[-L_i, L_i]$ by X^i (resp. the first exit time from $[-L_i, L_i]$ by X^i given $\{X^i_{\tau_i} = \pm L_i\}$).

Thanks to these expressions, $M_{0,1}(T, z)$ and $M_{i,\eta}(\theta, z)$ are easily computed, since

$$\begin{aligned}
&\mathbb{P}_{x_j}[X^j_\theta = z_j, \tau^j > T] = p^j(\theta, x_j, z_j),\\
&\mathbb{P}_{x_i}[\tau_i = \theta, X^i_\theta = \pm L_i] = q^{i,\pm}(\theta, x_i)\Phi^{i,\pm}(x_i) \text{ if } (i,-1) \in \mathfrak{A} \text{ and } (i,1) \in \mathfrak{A},\\
&\mathbb{P}_{x_i}[\tau_i = \theta, X^i_\theta = L_i] = q^i(\theta, x_i) \text{ if } (i,-1) \in \mathfrak{R} \text{ and } (i,1) \in \mathfrak{A},\\
&\mathbb{P}_{x_i}[\tau_i = \theta, X^i_\theta = -L_i] = q^i(\theta, x_i) \text{ if } (i,-1) \in \mathfrak{A} \text{ and } (i,1) \in \mathfrak{R}.
\end{aligned}$$

3 Analytical expressions for the densities

In order to compute $p^i(t, x, y)$ and then $q^i(t, x)$ and $q^{i,\pm}(t, x)$ by (6) and (7), one has to solve (5). Using a scaling principle, we may indeed assume that $L_i = 1$, as

$$p^i(t, x, y) = \frac{1}{L_i} p\left(\frac{t}{L_i^2}, \frac{x}{L_i}, \frac{y}{L_i}; L_i\mu\right),$$

where $p(t,x,y;\nu)$ is solution to (5) with $L_i = 1$ and a convective term μ_i equal to ν.

There are basically two ways to obtain $p(t,x,y;\nu)$. The first one is based on the spectral expansion of $\frac{1}{2}\triangle + \nu\nabla$, since this operator may be reduced to a self-adjoint one with respect to the scalar product induced by the measure $\exp(-2\nu x)$. The second one is the method of images when $\nu = 0$. If $\nu \neq 0$, the case of a Dirichlet boundary condition at both endpoints may be treated by using a simple transform that reduces the problem to $\nu = 0$. For the case of Neumann boundary condition at both endpoints, one can invert term by term the Laplace transform of a series giving the Green function. In the case of a mixed boundary condition, this method gives rise to series that cannot be used in practice, so only the spectral expansion should be used. In addition, the first eigenvalues have to be computed numerically.

As the formula are standard in most of the cases, we give the relevant expressions in Appendix A.

4 Dealing with a general domain

We are interested in solving by a Monte Carlo method a parabolic or an elliptic PDE. The idea is to decompose the domain in the union of time-space parallelepipeds and to simulate the successive exit times and positions from these parallelepipeds which need to be carefully chosen in order to control the error made at each simulation.

4.1 From parallelepipeds to right parallelepipeds

We still use the notations of Section 2. We consider first the parabolic PDE with constant coefficients λ, c and $\mu = (\mu_i)_{i=1,\dots,d}$ on the rectangle R_T:

$$\begin{cases} \dfrac{\partial v(t,x)}{\partial t} + \dfrac{1}{2}\displaystyle\sum_{i=1}^{d} \dfrac{\partial^2 v(t,x)}{\partial x_i^2} + \sum_{i=1}^{d} \mu_i \dfrac{\partial v(t,x)}{\partial x_i} + cv(t,x) = \lambda \text{ on } R_T, \\ \dfrac{\partial v(t,x)}{\partial x_i} = 0 \text{ for } x \in S_{i,\eta} \text{ if } (i,\eta) \in \mathfrak{R} \cap [\![1,d]\!] \times \{-1,1\}, \\ v(t,x) = \phi(t,x) \text{ for } x \in S_{i,\eta} \text{ if } (i,\eta) \in \mathfrak{A} \cap [\![1,d]\!] \times \{-1,1\}, \\ v(T,x) = g(x) \text{ if } T < +\infty. \end{cases} \tag{8}$$

Let X be the diffusion process whose components are given by (2). We assume that a classical solution to this problem exists, which is for example the case if ϕ and g are continuous and bounded. Then it follows from the Itô

formula applied to X that, for $t \in [0,T]$,

$$v(t,x) = \mathbb{E}_x[e^{c(\tau-t)}\phi(\tau-t, X_{\tau-t})); \tau < T-t] \\ + \mathbb{E}_x[e^{c(T-t)}g(X_{T-t}); \tau = T-t] + \mathbb{E}_x\left[\lambda \int_0^{\tau-t} e^{c(\tau-t-s)}\,\mathrm{d}s\right],$$

where τ is the first exit time from R_T.

Let σ be an invertible $d \times d$-matrix. The function $u(t,x) = v(t,\sigma^{-1}x)$ is solution to

$$\begin{cases} \dfrac{\partial u(t,x)}{\partial t} + \dfrac{1}{2}\displaystyle\sum_{i,j=1}^{d} [\sigma\sigma^*]_{i,j} \frac{\partial^2 u(t,x)}{\partial x_i \partial x_j} \\ \qquad + \displaystyle\sum_{i=1}^{d} [\mu\sigma^*]_i \frac{\partial u(t,x)}{\partial x_i} + cu(t,x) = \lambda \text{ on } [0,T] \times \sigma R, \\ \sigma_{j,i}\dfrac{\partial u(t,x)}{\partial x_j} = 0 \text{ for } x \in \sigma S_{i,\eta} \text{ if } (i,\eta) \in \mathfrak{R} \cap [\![1,d]\!] \times \{-1,1\}, \\ u(t,x) = \phi(t,\sigma^{-1}x) \text{ for } x \in \sigma S_{i,\eta} \text{ if } \ (i,\eta) \in \mathfrak{A} \cap [\![1,d]\!] \times \{-1,1\}, \\ u(T,x) = g(\sigma^{-1}x) \text{ if } T < +\infty. \end{cases} \tag{9}$$

If $\mathbf{n}_i$ is a unit vector orthogonal to the side $\sigma S_{i,\eta}$, then $\mathbf{n}_i = (\sigma^*)^{-1}\mathbf{e}_i$, where $\mathbf{e}_i$ is the unit vector in the i-th direction. It follows that $\sigma\sigma^*\mathbf{n}_i = \sigma\mathbf{e}_i$ and thus

$$\text{for } x \in \sigma S_{i,\pm 1},\ [\sigma\sigma^*]\mathbf{n}_i \cdot \nabla u(t,x) = \sigma_{j,i}\frac{\partial u(t,x)}{\partial x_j},$$

which means that a Neumann boundary condition in the co-normal direction holds in (9) on $\sigma S_{i,\eta}$ if $(i,\eta) \in \mathfrak{R}$.

It is then possible to solve (9) by reducing the problem to (8) and use a Monte Carlo method to compute the values of $u(t,x)$.

4.2 The hypotheses

Let us consider a domain Q in $\mathbb{R}_+ \times \mathbb{R}^d$. For the sake of simplicity, we assume that Q is the cylinder $[0,T] \times D$ (with possibly $T = +\infty$), where D is an open, bounded domain of $\mathbb{R}^d$ with piecewise smooth boundary. Let us consider a function a with values in the space of $d \times d$-symmetric matrices which is continuous on D and everywhere positive definite, together with some functions $b : Q \to \mathbb{R}^d$, $c : Q \to \mathbb{R}$ and $f : Q \to \mathbb{R}$. For all $(t,x) \in Q$, we denote by $\sigma(t,x)$ a $d \times d$-symmetric matrix such that $\sigma(t,x)\sigma^*(t,x) = a(t,x)$.

We set

$$L = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}(t,x)\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i(t,x)\frac{\partial}{\partial x_i}. \tag{10}$$

We give below some hypotheses under which we will establish the convergence of the algorithm. However, we do not claim that these hypotheses are optimal. Basically, to set up a Monte Carlo numerical scheme, one needs three ingredients, that are inter-related:

(i) The existence and the uniqueness of a solution u to

$$\begin{cases} \dfrac{\partial u(t,x)}{\partial t} + Lu(t,x) + c(t,x)u(t,x) + f(t,x) = 0 \text{ on } [0,T] \times D, \\ u(T,x) = g(x), \ x \in D, \\ u(t,x) = \phi(t,x) \text{ on } \Gamma_{\mathrm{d}} \subset [0,T) \times \partial D, \\ \partial_n u(t,x) = 0 \text{ on } \Gamma_{\mathrm{n}} \subset [0,T) \times \partial D, \end{cases} \tag{11}$$

where ∂_n denotes the co-normal derivative along the lateral surface, and Γ_{d} (resp. Γ_{n}) are subsets of $[0,T) \times \partial D$ on which a Dirichlet (resp. Neumann) boundary condition hold.

(ii) The existence of a solution to the diffusion process associated to L. Note that since the simulation involves distributions and not stochastic integrals, we do not need strong existence for the associated SDE.

(iii) That the solution u is given in term of the probabilistic representation

$$\begin{aligned} u(t,x) = \mathbb{E}_{t,x} \left[\exp\left(\int_t^\tau c(s,X_s)\,\mathrm{d}s \right) \phi(\tau, X_\tau) \mathbb{1}_{\tau<T} \right] \\ + \mathbb{E}_{t,x} \left[\exp\left(\int_t^T c(s,X_s)\,\mathrm{d}s \right) g(X_T) \mathbb{1}_{\tau>T} \right] \\ + \mathbb{E}_{t,x} \left[\int_t^{\tau \wedge T} \exp\left(\int_t^s c(r,X_r)\,\mathrm{d}r \right) f(s,X_s)\,\mathrm{d}s \right], \end{aligned} \tag{12}$$

where τ is the first exit time from $[0,+\infty) \times D$ by a point of Γ_d.

Notation 1. We denote by $\mathcal{P}$ the set of time-space parallelepipeds P such that there exist $0 \le s < t \le T$, $L_1, \ldots, L_d$, $x \in \mathbb{R}^d$ such that

$$P = [s,t] \times (x + \widehat{\sigma}([-L_1, L_1] \times \cdots \times [-L_d, L_d])),$$

where $\widehat{\sigma}$ is a $d \times d$-matrix. Possibly $t = +\infty$ (if $T = +\infty$).

Our assumptions are the following:

(H1) There exists a subset $\mathcal{P}_D$ of $\mathcal{P}$ such that $Q = \cup_{P \in \mathcal{P}_D} P$. Besides, if $P = [s,t] \times U \in \mathcal{P}$ for a parallelepiped U, then for all $r \in [s,t)$, $[r,t] \times U \in \mathcal{P}$. In other words, one can truncate the parallelepipeds in time.

(H2) There exist $\Gamma_{\rm n}$, $\Gamma_{\rm d}$ contained in $\partial Q = [0,T]\times\partial D$ and some subsets $\mathcal{P}_{\rm n}$, $\mathcal{P}_{\rm d}$ of I such that $\Gamma_{\rm n}\subset\cup_{P\in\mathcal{P}_{\rm n}}\partial P$, $\Gamma_{\rm d}\subset\cup_{P\in\mathcal{P}_{\rm d}}\partial P$, the closure of $\Gamma_{\rm n}\cup\Gamma_{\rm d}$ is equal to $[0,T]\times\partial D$ and $\Gamma_{\rm n}\cap\Gamma_{\rm d}=\emptyset$. This means that the boundary of $[0,T]\times\partial D$ is decomposed in two parts, where either the Dirichlet or the Neumann boundary conditions hold. This hypothesis means that a side of a parallelepiped in $\mathcal{P}_D$ contained in ∂Q is contained either in $\Gamma_{\rm n}$ or in $\Gamma_{\rm d}$.

(H3) The differential operator L is the generator of a continuous diffusion process X that is reflected at $\Gamma_{\rm n}$ and killed when reaching $\Gamma_{\rm d}\cup\{T\}\times D$, and the probabilistic representation of the solution given by (12) holds (see for example [LS84] for existence results of such reflected process, and [SV79] if there are no reflections).

(H4) There exists an unique solution u of class $\mathcal{C}^{1,2}$ on $[0,T)\times D$ to (11) which is continuous on $[0,T]\times\overline{D}$.

(H5) To $P=[s,t]\times(x+\widehat{\sigma}R)\in\mathcal{P}_D$ for a right parallelepiped R and a matrix $\widehat{\sigma}$, we associate a vector $\widehat{b}\in\mathbb{R}^d$, two constants $\widehat{c}$, $\widehat{f}$ and we construct the differential operator

$$\widehat{L}=\frac{1}{2}\sum_{k,l=1}^{d}\widehat{a}_{k,\ell}\frac{\partial^2}{\partial x_k\partial x_\ell}+\sum_{k=1}^{d}\widehat{b}_k\frac{\partial}{\partial_{x_k}}$$

with $\widehat{a}=\widehat{\sigma}\widehat{\sigma}^*$.

Fix $\varepsilon>0$. We assume that the solution u to (11) satisfies for any y in the interior of $x+\widehat{\sigma}R$,

$$\mathbb{E}_{s,y}\left|\int_s^\tau e^{\widehat{c}(r-s)}\left(\frac{\partial u}{\partial t}+\widehat{L}u+\widehat{c}u-\widehat{f}\right)(r,\widehat{X}_r)\,\mathrm{d}r\right|\leq\varepsilon \tag{13}$$

where $\widehat{X}$ is the diffusion process generated by $\widehat{L}$ and τ is its first exit time from P.

Remark 2. If $T=+\infty$ and, the coefficients are time-homogeneous and $\Gamma_{\rm d}=[0,\infty)\times\gamma_{\rm d}$, $\Gamma_{\rm n}=[0,\infty)\times\gamma_{\rm n}$, then $v(x)=u(0,x)$ is solution to the elliptic PDE

$$\begin{cases}Lv(x)+c(x)v(x)=f(x)\text{ on }D,\\ v(x)=\phi(x)\text{ on }\gamma_{\rm d}\subset\partial D,\\ \partial_n v(x)=0\text{ on }\gamma_{\rm n}\subset\partial D.\end{cases} \tag{14}$$

Thus, by solving the parabolic PDE (11), we may also solve the elliptic PDE (14), and we focus only on (11).

Remark 3. The problem of the existence of a stochastic process reflected on some part of the boundary of $[0,T)\times D$ is deduced from the existence of a stochastic process reflected on the lateral boundary $[0,T)\times D$, which is killed when it reaches $\Gamma_{\rm n}$.

4.3 The algorithm and its weak error

In order to simplify the notations, if $T<+\infty$, we denote the final condition g of (11) by $\phi(T,x)$.

Given $(t,x)\in Q$, the solution $u(t,x)$ of (11) is computed by the Feynman-Kac formula. For this, we have to simulate the diffusion process X up to its first exit time τ from Q (with the implicit convention that the particle cannot exit by a piece of boundary where a Neumann b.c. holds). Let u be the solution of (11) and perform the following notations

$$\text{for } s\geq t,\ \begin{cases} Y_s = 1+\displaystyle\int_t^s c(r,X_r)Y_r\,\mathrm{d}r = \exp\left(\int_t^s c(r,X_r)\,\mathrm{d}r\right), \\ Z_s = \displaystyle\int_t^s f(r,X_r)Y_r\,\mathrm{d}r. \end{cases}$$

Then $u(t,x)$ is then given by

$$u(t,x)=\mathbb{E}_{t,x}[\phi(\tau,X_\tau)Y_\tau+Z_\tau]. \tag{15}$$

We construct now the algorithm that approximates (15) by a Monte Carlo method.

Algorithm 2. Assume that we are initially at the point $(t,x)\in Q$ and fix a number N of particles.

(1) For $i=1,\dots,N$ do
  (A) Set $(\theta_0,\Xi_0,Y_0,Z_0,W_0)=(t,x,1,0,1)$ and $k=0$.
  (B) Repeat
    (a) Choose an element $P^{(k)}\in\mathcal{P}_D$ of the form $P^{(k)}=[\theta_k,s]\times U$, $U\subset\mathbb{R}^d$ such that (θ_k,Ξ_k) belongs to the basis of P (s is possibly infinite if for example $T=+\infty$ and the coefficients are time-inhomogeneous). On $P^{(k)}$, consider the differential operator $L^{(k)}$ as well $c^{(k)}$ and $f^{(k)}$ which approximate L, c and f as in (H5).
    (b) Draw a realization of a random variable (θ_{k+1},Ξ_{k+1}) with values in $(\{s\}\times U)\cup((\theta_k,s)\times\partial U)$ and compute its associated weight w_k as shown in Sections 2 and 4.1 by considering the exit time and position from the parallelepiped $P^{(k)}$.

(c) Compute $W_k = W_{k-1} w_k$ and

$$Y_{k+1} = Y_k \exp(c^{(k)}(\theta_{k+1} - \theta_k))$$
$$Z_{k+1} = Z_k + f^{(k)} \int_{\theta_k}^{\theta_{k+1}} \exp(c^{(k)} s)\, \mathrm{d}s.$$

(d) If $\Xi_{k+1} \in \Gamma_{\mathrm{d}}$ or $\theta_{k+1} = T$, then exit from the loop.

(e) Increase k.

(C) Set $(\theta^{(i)}, \Xi^{(i)}, Y^{(i)}, Z^{(i)}, W^{(i)}) = (\theta_{k+1}, \Xi_{k+1}, Y_{k+1}, Z_{k+1}, W_k)$.

(2) Return

$$\widehat{u}(t,x) = \frac{1}{N} \sum_{i=1}^{N} \left(W^{(i)} \phi(\theta^{(i)}, \Xi^{(i)}) Y^{(i)} + W^{(i)} Z^{(i)} \right) \tag{16}$$

We denote by $\widehat{\mathbb{P}}$ the distribution of the Markov chain (θ_k, Ξ_k). Note that $(Y_k, Z_k, w_k)_{k \geq 0}$ is constructed from $(\theta_k, \Xi_k)_{k \geq 0}$.

Proposition 2. *For any $(t,x) \in [0,T) \times D$,*

$$|u(t,x) - \widehat{\mathbb{E}}[\widehat{u}(t,x)]| \leq \varepsilon \widehat{\mathbb{E}} \left[W_\nu \nu \exp(M \theta_\nu) \right], \tag{17}$$

where ε is defined in (H5), ν is the number of steps that $(\theta_k, \Xi_k)_{k \geq 0}$ takes to reach the boundary $\Gamma_{\mathrm{d}} \cap \{T\} \times D$ and

$$M = \sup_{(s,y) \in [t,T) \times D} c(s,y).$$

Remark 4. Note that the weak error in (17) does not depend on the choice of the importance sampling technique. However, the Monte Carlo error depends on this choice. In addition, if the coefficients a, b, f and c are constant on the domain, then one may choose $\varepsilon = 0$ and the simulation is exact.

Proof. To the Markov chain (θ_k, Ξ_k) is also associated a random sequence of parallelepipeds $(P^{(k)})_{k=0,\ldots,\nu}$. We denote by τ_k the successive times the diffusion process X reaches the boundary of the $P^{(k)}$'s.

Since $Z_0 = 0$, $Y_0 = 1$ and $u = \phi$ on the boundary of Q,

$$\begin{aligned} \widehat{\mathbb{E}}[\widehat{u}(t,x)] &= \widehat{\mathbb{E}}[W_\nu Y_\nu \phi(\theta_\nu, \Xi_\nu) + W_\nu Z_\nu] \\ &= u(t,x) + \widehat{\mathbb{E}} \left[W_\nu \sum_{k=0}^{\nu-1} (Z_{k+1} - Z_k + Y_{k+1} u(\theta_{k+1}, \Xi_{k+1}) - Y_k u(\theta_k, \Xi_k)) \right]. \end{aligned} \tag{18}$$

Let $(\mathcal{G}_k)_{k \geq 0}$ be the filtration generated by the Markov chain $(\theta_k, \Xi_k)_{k \geq 0}$. We remark that Y_k and Z_k are measurable with respect to $\mathcal{G}_k$, while w_k

is measurable with respect to $\mathcal{G}_{k+1}$ (since it is computed from θ_k, Ξ_k, θ_{k+1} and Ξ_{k+1}).

By using the Markov property, after setting $W_{k+1,\nu} = \widehat{\mathbb{E}}[w_{k+1}\cdots w_\nu \,|\, \mathcal{G}_{k+1}]$, we get

$$\begin{aligned}
&\widehat{\mathbb{E}}[W_n(Z_{k+1}-Z_k)] = \widehat{\mathbb{E}}[W_{k+1,\nu}\widehat{\mathbb{E}}[w_k(Z_{k+1}-Z_k)\,|\,\mathcal{G}_k]W_{k-1}],\\
&\widehat{\mathbb{E}}[W_\nu(Y_{k+1}u(\theta_{k+1},\Xi_{k+1}) - Y_k u(\theta_k,\Xi_k))]\\
&\quad = \widehat{\mathbb{E}}[W_{k+1,\nu}\widehat{\mathbb{E}}[w_k(Y_{k+1}u(\theta_{k+1},\Xi_{k+1}) - Y_k u(\theta_k,\Xi_k))\,|\,\mathcal{G}_k]W_{k-1}].
\end{aligned}$$

Let us denote by $(X^{(k)}, \mathbb{P}^{(k)}_{t,x})$ the process generated by the operator $L^{(k)}$ with constant coefficients $a^{(k)}$ and $b^{(k)}$ on $P^{(k)}$. Define recursively $(t^{(0)}, x^{(0)}) = (t,x)$ and $(t^{(k+1)}, x^{(k+1)}) = (\tau^{(k)}, X^{(k)}_{\tau^{(k)}})$, where $\tau^{(k)}$ is the first exit time from $P^{(k)}$ for the diffusion $X^{(k)}$. Let also $f^{(k)}$ and $c^{(k)}$ be the values we choose to approximate f and c on $P^{(k)}$, and define also recursively $y^{(0)} = 1$ and $y^{(k)} = y^{(k-1)}\exp(c^{(k)}(t^{(k+1)} - t^{(k)}))$.

Thus, from the construction of $\widehat{\mathbb{P}}$ and the Itô formula,

$$\begin{aligned}
&\widehat{\mathbb{E}}[w_k(Y_{k+1}u(\theta_{k+1},\Xi_{k+1}) - Y_k u(\theta_k,\Xi_k))\,|\,\mathcal{G}_k]\\
&\quad = y^{(k)}\mathbb{E}^{(k)}_{t^{(k)},x^{(k)}}[(e^{c^{(k)}(t^{(k+1)}-t^{(k)})}u(t^{(k+1)}, X^{(k+1)}_{t^{(k+1)}}) - u(t^{(k)},x^{(k)}))]\\
&\quad = y^{(k)}\mathbb{E}^{(k)}_{t^{(k)},x^{(k)}}\left[\int_{t^{(k)}}^{t^{(k+1)}} e^{c^{(k)}(s-t^{(k)})}\left(\frac{\partial}{\partial t} + L^{(k)} + c^{(k)}\right)u(s, X^{(k)}_s)\,\mathrm{d}s\right].
\end{aligned}$$

Also,

$$\widehat{\mathbb{E}}[w_k(Z_{k+1}-Z_k)\,|\,\mathcal{G}_k] = y^{(k)}\mathbb{E}^{(k)}_{t^{(k)},x^{(k)}}\left[f^{(k)}\int_{t^{(k)}}^{t^{(k+1)}} e^{c^{(k)}s}\,\mathrm{d}s\right].$$

It follows from our hypotheses on the choice of the coefficients and the parallelepiped $P^{(k)}$ that

$$\begin{aligned}
&\left|\widehat{\mathbb{E}}[w_k(Y_{k+1}u(\theta_{k+1},\Xi_{k+1}) - Y_k u(\theta_k,\Xi_k) + Z_{k+1} - Z_k)\,|\,\mathcal{G}_k]\right|\\
&= \left|y^{(k)}\mathbb{E}^{(k)}_{t^{(k)},x^{(k)}}\left[\int_{t^{(k)}}^{t^{(k+1)}} e^{c^{(k)}(s-t^{(k)})}\left(\left(\frac{\partial}{\partial t} + L^{(k)} + c^{(k)}\right)u(s,X^{(k)}_s) + f^{(k)}\right)\,\mathrm{d}s\right]\right|\\
&\qquad\qquad \le y^{(k)}\varepsilon \le \widehat{\mathbb{E}}\left[\varepsilon w_k Y_k\,|\mathcal{G}_k\right],
\end{aligned}$$

since the Y_k's (and then the $y^{(k)}$'s) are positive. Hence, from (18) and then Jensen inequality applied to $|\cdot|$,

$$|\widehat{\mathbb{E}}[Y_\nu\phi(\theta_\nu,\Xi_\nu) + Z_\nu] - \widehat{\mathbb{E}}[\widehat{u}(t,x)]| \le \varepsilon\widehat{\mathbb{E}}\left[W_\nu\sum_{k=0}^{\nu-1}Y_k\right].$$

As $0 < Y_k \leq e^{M\theta_k}$ for $k = 0, \ldots, \nu$, we obtain (17). $\square$

4.4 The Monte Carlo error

In order to compute the solution $u(t,x)$ of (11), we have constructed the estimator $\widehat{u}(t,x)$ given by (16), whose variance is

$$\mathrm{Var}_{\widehat{\mathbb{P}}}\,\widehat{u}(t,x) = \frac{1}{N}\,\mathrm{Var}_{\widehat{\mathbb{P}}}(W_\nu \phi(\theta_\nu, \Xi_\nu) Y_\nu + W_\nu Z_\nu).$$

The Monte Carlo error depends of course of this variance $\sigma^2 = \mathrm{Var}_{\widehat{\mathbb{P}}}\,\widehat{u}(t,x)$, since asymptotically for $N \to \infty$ the true mean $\widehat{\mathbb{E}}[\widehat{u}(t,x)]$ lies in the interval $[\widehat{u}(t,x) - 2\sigma, \widehat{u}(t,x) + 2\sigma]$ with a confidence of 99 %.

We denote by $\widehat{\mathbb{P}}^{\mathrm{n}}$ the distribution of $(\theta_k, \Xi_k)_{k\geq 0}$ when we use the real distribution of the exit time and position of the rectangles, which means that the weights are equal to 1. Any event Φ measurable with respect to $(\theta_k, \Xi_k)_{k\geq 0}$ satisfies $\widehat{\mathbb{P}}^{\mathrm{n}}[\Phi] = \widehat{\mathbb{P}}[W\Phi]$.

We then get

$$\mathrm{Var}_{\widehat{\mathbb{P}}}(W_\nu \phi(\theta_\nu, \Xi_\nu) Y_\nu + W_\nu Z_\nu) = \Psi + \mathrm{Var}_{\widehat{\mathbb{P}}^{\mathrm{n}}}(\widehat{u}(t,x)).$$

with

$$\Psi = \widehat{\mathbb{E}}^{\mathrm{n}}[(W_\nu - 1)(\phi(\theta_\nu, \Xi_\nu) Y_\nu + Z_\nu)^2]$$

Thus, a good choice of the density for the exit time and position from the parallelepipeds is one for which $\Psi \leq 0$ and as small as possible. However, reducing the variance is a difficult task, and motivates the need of some automatic selection/optimization techniques, as explained in the introduction part.

In addition, the numerical experiments we performed up to now highlight another difficulty, which comes from the fact that W_ν may take large values, which implies meaningless values for $\widehat{u}(t,x)$. That is why we suggest to keep track also of the empirical distribution, or at least the variance of W_ν.

To illustrate this point, let us assume that the diffusion process X has no drift and that for the simulation, the right parallelepipeds we use are squares centered on the particle, each time with the same density for the exit time and position. By a scaling argument, the distribution of the weight w_k at the k-th step does not depend on the size of the squares, so that the w_k's are independent and identically distributed under $\widehat{\mathbb{P}}$.

We set $\xi^i = \log(w_i)$, so that $W_n = \exp\left(\sum_{i=1}^n \xi^i\right)$. As the ξ^i are independent and identically distributed, we assume that, if $S_n = \sum_{i=1}^n \xi^i$, then $S_n/\sqrt{n}$ converges to some normal random variable χ with mean μ and variance σ^2, so that, for n large enough, the distribution of W_n is close to the

one of $\exp(\sqrt{n}\chi)$. Thus, with the expression of the Laplace transform of the normal distribution, for $\kappa = 1, 2$,

$$\widehat{\mathbb{E}}[(W_n)^\kappa] \approx \mathbb{E}[\exp(\kappa\sqrt{n}\chi)] = \exp\left(\mu\kappa\sqrt{n} + n\frac{\kappa^2\sigma^2}{2}\right).$$

Hence, we get that

$$\begin{aligned}\mathrm{Var}_{\widehat{\mathbb{P}}}(W_n) &\approx \exp\left(2\mu\sqrt{n} + 2n\sigma^2\right) - \exp\left(\mu\sqrt{n} + \frac{n}{2}\sigma^2\right)\\ &\approx \exp(2n\sigma^2)\left(\exp\left(\frac{\mu}{\sqrt{n}} + 1\right) - \exp\left(\frac{\mu}{2\sqrt{n}} - \frac{3n}{2}\sigma^2\right)\right)\\ &\underset{n\to\infty}{\sim} \exp(1 + 2n\sigma^2).\end{aligned}$$

Thus, when n becomes too large, the variance of W_n explodes, while $\widehat{\mathbb{E}}[W_n] = 1$ for any $n \geq 1$.

In [GI89] (see also [Gla04]), P. Glynn and D. Iglehart exhibit another argument that shows the simulation performs badly if too much steps are used.

4.5 Estimation of the number of steps

We can now turn to the estimation of the number of steps. We use for this the techniques employed in [Mil95, MT99, MT04].

In Algorithm 2, we have constructed a Markov chain $(\Lambda_k)_{k\geq 0}$ with $\Lambda_k = (\theta_k, \Xi_k)$ which is absorbed when reaching $\Gamma_{\mathrm{k}} = \Gamma_{\mathrm{d}} \cap \{T\} \times D$.

For a function u on D, we set

$$Pu(t,x) = \widehat{\mathbb{E}}^{\mathrm{n}}[u(\Lambda_1) \,|\, \Lambda_0 = (t,x)] \text{ and } A = Pu(t,x) - u(t,x).$$

The latter operator is the generator of a Markov chain.

Lemma 1. *If $T < +\infty$ and*

$$\widehat{\mathbb{E}}^{\mathrm{n}}[\theta_1 \,|\, (\theta_0, \Xi_0) = (t,x)] - t \geq \gamma,$$

then

$$\widehat{\mathbb{E}}^{\mathrm{n}}[\nu \,|\, (\theta_0, \Xi_0) = (t,x)] \leq 1 + \frac{T-t}{\gamma}.$$

Proof. We consider the problem

$$\begin{cases} Av(t,x) = -g(t,x) \text{ on } Q,\\ u(t,x) = 0 \text{ on } [0,T] \times \Gamma \end{cases}$$

whose solution is

$$u(t,x) = \widehat{\mathbb{E}}^{\mathrm{n}}\left[\sum_{k=0}^{\nu-1} g(\Lambda_k)\right].$$

Thus, one can get a good estimate of $\widehat{\mathbb{E}}^{\mathrm{n}}[\nu]$ if u and g are well chosen.

Let $V(t,x)$ be the function $V(t,x) = (T-t)\mathbb{1}_{(t,x)\in Q}$. So, for (t,x) in Q,

$$AV(t,x) = \widehat{\mathbb{E}}^{\mathrm{n}}[V(\theta_1,\Xi_1)\,|\,(\theta_0,\Xi_0) = (t,x)] - (T-t) \leq -\gamma.$$

Hence $T - t \geq \widehat{\mathbb{E}}^{\mathrm{n}}[\sum_{k=0}^{\nu-1}\gamma\,|\,(\theta_0,\Xi_0) = (t,x)]$ and the result follows easily. □

Lemma 2. *With the previous notations, for every $L > 0$,*

$$\sup_{x\in Q} \widehat{\mathbb{P}}^{\mathrm{n}}\left[\nu \geq L | (\theta_0,\Xi_0) = (t,x)\right] \leq (1+T-t)\exp(-c\gamma L/(1+T-t))$$

for some constant c that converges to 1 as γ decreases to 0.

Proof. The proof is similar to the one in Theorem 7.2 in [MT99]. □

Lemma 3. *If $T = +\infty$, Q is bounded and*

$$\widehat{\mathbb{E}}^{\mathrm{n}}[|x+\Xi_1+c|^2] \geq \gamma > 0,$$

where c is such that $\min_{x\in\overline{Q}}|x+c| \geq C > 0$. Then

$$\widehat{\mathbb{E}}^{\mathrm{n}}[\nu] \leq \frac{B^2 - C^2}{B^2 - \gamma}$$

with $B > \max\{\gamma, \sup_{x\in\overline{Q}}|x+c|\}$.

Proof. Here again, we proceed as in [Mil95]. We choose a vector c such that $\min_{x\in\overline{Q}}|x+c| \geq C > 0$ and set

$$V(t,x) = \begin{cases} B^2 - |x+c|^2 & \text{if } (t,x)\in\mathbb{R}_+\times Q, \\ 0 & \text{otherwise.} \end{cases}$$

Hence, if $B^2 > \gamma$,

$$AV(t,x) \leq |x+c|^2 - \widehat{\mathbb{E}}^{\mathrm{n}}[|x+\Xi_1+c|^2\,|\,(\theta_0,\Xi_0) = (t,x)] \leq B^2 - \gamma$$

and the result follows. □

5 Numerical examples

We present in this Section four numerical tests which illustrate our algorithm.

5.1 Speeding up the random walk on squares algorithm

In [MT99] (see also [MT04]), G.N. Milstein and M.V. Tretyakov proposed a method to simulate Brownian motions and solutions of SDEs by using the first exit time and position (τ, B_τ) from a hyper-cube or a time-space parallelepiped with cubic space basis. This is a variation of the method of random walk on spheres. Although some authors already used random walk on squares and rectangles by using the explicit expression of the Green function and without simulating the exit time (see for example [SM04]), one of the main feature of this approach is the simulation of the couple of non-independent random variables (τ, B_τ) by simulating real valued random variables (we have explained in [DL06] how to extend this approach to rectangles for any starting point, still using one-dimensional distributions).

Yet the drawback of this approach is that it is rather time consuming unless tabulated functions are used, since one has to invert the distribution function of the first exit time $\tau_{-1,1}$ from $[-1,1]$ for the Brownian motion, and then the distribution function $P(y) = \mathbb{P}_0[B_t < y \,|\, t < \tau_{-1,1}]$, where W is a one-dimensional Brownian motion. Analytical expressions for these distribution function are easily deduced from the series we gave in Appendix A.

We are looking now how to speed up the computations by using a simple density for the exit position. This also allows us to illustrate the point of Section 4.4.

We consider the d-dimensional hypercube $C = [-1,1]^d$, and a fixed time $T > 0$ (possibly $T = +\infty$). Let B be a d-Brownian motion. We set $\tau = \inf\{t > 0 \,|\, B_t \notin C\}$. Let W be a one-dimensional Brownian motion. We set $\tau_{-1,1} = \inf\{t > 0 \,|\, W_t \notin [-1,1]\}$, $Q(t) = \mathbb{P}_0[\tau_{-1,1} < t]$, $P(t,y) = \mathbb{P}_0[W_t < y \,|\, t < \tau_{-1,1}]$, $q(t) = Q'(t)$ and $p(t,y) = \partial_y P(t,y)$.

Let us note that one can easily pass from $C = [-1,1]^d$ to any hypercube $[-L,L]^d$ after a proper scaling argument on space and time. Thus, from a numerical point of view, one only needs to implement the required functions p, q, P and Q on $[-1,1]$.

To simulate the exit time and position from $[0,T] \times C$, we perform in the following steps:

- Compute the probability $\alpha = 1 - (1 - Q(T))^d$ that $\tau < T$.
- If $\tau < T$,
  - For a realization U of a uniform random variable U on $[0,1)$, set
$$\overline{\tau} = Q^{-1}(1 - (1 - \mathsf{U}\alpha)^{1/d}).$$
    which is a realization of τ given $\{\tau < T\}$.
  - Choose with probability $1/2d$ an exit side (J, ε) and set $\xi_J = \varepsilon$.

- For each $i = 1, \dots, d$, $i \neq J$, set $\chi_i = \sqrt{\mathsf{U}_i}$, where the U_i's are $d-1$ independent realizations of u. With probability $1/2$, set $\xi_i = \chi_i - 1$ and with probability $1/2$, set $\xi_i = 1 - \chi_i$.
- Compute the weight

$$w = \frac{1}{1 - Q(\overline{\tau})} \prod_{i=1,\dots,d, i \notin J} \frac{p(\overline{\tau}, \xi_i)}{\chi_i}.$$

- If $\tau > T$, then
  - Set $\overline{\tau} = T$.
  - For $i = 1, \dots, d$, set $\chi_i = \sqrt{\mathsf{U}_i}$, where the U_i's are $d-1$ independent realizations of u. With probability $1/2$, set $\xi_i = \chi_i - 1$ and with probability $1/2$, set $\xi_i = 1 - \chi_i$.
  - Compute then the weight

$$w = \frac{1}{1 - \alpha} \prod_{i=1,\dots,d} \frac{p(T, \xi_i)}{\chi_i}.$$

Hence $(\overline{\tau}, \xi_1, \dots, \xi_d)$ represent the first exit time and position from $[0, T] \times C$, and w is the associated weight.

If the Brownian motion reaches the side labelled by $(1, -1)$ first at time τ, then we use for simulating B_t^i for $i = 2, \dots, d$ a random variable with density $\phi(x) = 1 + x$ if $x \in (-1, 0]$ and $\phi(x) = 1 - x$ if $x \in [0, -1)$, that are very simple to simulate. Indeed, the weights w are close to 1 as we see in Table 1, and the execution time is divided by 2. However, for $T = 0.1$, the variance of w is too high and leads to some instabilities. In this case, it is preferable to simulate the exact distributions of B_T given $\{T \leq \tau\}$.

Method	T	mean of w	variance of w	time (s)
Walk on squares	0.1	–	–	141
Imp. Sampling	0.1	0.9993	0.2825	49
Walk on squares	0.5	–	–	141
Imp. Sampling	0.5	0.9999	0.0215	49
Walk on squares	1.0	–	–	137
Imp. Sampling	1.0	0.9999	0.0175	63
Walk on squares	$+\infty$	–	–	124
Imp. Sampling	$+\infty$	0.9998	0.0153	60

Table 1: Speeding up the random walk on squares: experiments with 1.000.000 samples are used.

5.2 Solving a bi-harmonic problem

To test the validity of our approach with respect to other algorithms, we consider first an example borrowed in [MT99] (see also [MT04, p. 332]). Let $D = [-1, 1]^2$, and consider the bi-harmonic equation

$$\begin{cases} \frac{1}{2}\triangle^2 u(x) = 1, \ x \in D, \\ u(x) = \phi(x) \text{ on } \partial D, \\ \frac{1}{2}\triangle u(x) = \psi(x) \text{ on } \partial D \end{cases} \tag{19}$$

with

$$\phi(x_1, \pm 1) = \frac{1 + x_1^4}{12}, \ \phi(\pm 1, x_2) = \frac{1 + x_2^4}{12}, \tag{20}$$

$$\psi(x_1, \pm 1) = \frac{1 + x_1^2}{2}, \ \psi(\pm 1, x_2) = \frac{1 + x_2^2}{2}. \tag{21}$$

Setting $v(x) = \frac{1}{2}\triangle u(x)$, (19) may be transformed into the system

$$\begin{cases} \frac{1}{2}\triangle v(x) = 1 \text{ on } D \text{ with } u(x) = \psi(x) \text{ on } \partial D, \\ \frac{1}{2}\triangle u(x) - v(x) = 0 \text{ on } D \text{ with } u(x) = \phi(x) \text{ on } \partial D, \end{cases}$$

whose exact solution is

$$u(x) = \frac{x_1^4 + x_2^4}{12}, \ v(x) = \frac{x_1^2 + x_2^2}{2}.$$

By Itô formula, it is easy to show that

$$\begin{aligned} u(x) &= \mathbb{E}[\phi(x + B_\tau)] - \mathbb{E}[\tau\psi(x + B_\tau)] + \frac{1}{2}\mathbb{E}[\tau^2], \\ v(x) &= \mathbb{E}[\psi(x + B_\tau)] - \mathbb{E}[\tau], \end{aligned}$$

where B is a Brownian motion, and τ is its first exit time from D.

Here, in contrast with the values presented in [MT99], we only need to use one square, since we are not forced to start from its center. We compare the results given by our algorithm (first lines) with the one given by the random walk on rectangles (second line). Each side is chosen uniformly with probability 1/4. The time is drawn by using an exponential random variable of parameter $1/(1 - \varepsilon x_i)$ if (i, ε) is the exit side. The position is drawn uniformly on the exit side. This corresponds in some sense to a "naive" and simple way to choose the exit time and position.

As we evaluate quantities of the form $\mathbb{E}[f(\tau, B_\tau)]$, we report the quantities $\mu_n \pm 2\sigma_n/\sqrt{n}$, where μ_n is the empirical mean of $f(\tau, B_\tau)$ with n samples,

and σ_n is the corresponding empirical standard deviation. The interval $[\mu_n - 2\sigma_n/\sqrt{n}, \mu_n + 2\sigma_n/\sqrt{n}]$ represents the 99 % confidence interval for $\mathbb{E}[f(\tau, B_\tau)]$. The estimation $\overline{u}(x)$ and $\overline{v}(x)$ of u and v for three points are given in Table 2.

x	n	$u(x)$	$\overline{u}(x)$	$v(x)$	$\overline{v}(x)$	time (s)
$(0.3, 0.5)$	10^4	0.00588	0.0047 ± 0.0037	0.17000	0.1638 ± 0.0081	< 1
			0.0064 ± 0.0039		0.1684 ± 0.0081	8
—	10^5	—	0.0061 ± 0.0012	—	0.1669 ± 0.0026	1
			0.0062 ± 0.0012		0.1679 ± 0.0026	80
—	10^6	—	0.0059 ± 0.0004	—	0.1698 ± 0.0008	7
			0.0059 ± 0.0004		0.1696 ± 0.0008	750
$(0.7, 0.8)$	10^4	0.05414	0.0480 ± 0.0017	0.56500	0.5297 ± 0.0064	< 1
			0.0553 ± 0.0020		0.5707 ± 0.0061	17
—	10^5	—	0.0526 ± 0.0005	—	0.5593 ± 0.0019	1
			0.0543 ± 0.0006		0.5652 ± 0.0019	170
—	10^6	—	0.0536 ± 0.0002	—	0.5654 ± 0.0006	7
			0.0542 ± 0.0002		0.5650 ± 0.0006	1650
$(0.9, 0.9)$	10^4	0.10935	0.1103 ± 0.0009	0.81000	0.8186 ± 0.0034	< 1
			0.1109 ± 0.0020		0.8105 ± 0.0038	30
—	10^5	—	0.1131 ± 0.0002	—	0.8390 ± 0.0006	1
			0.1095 ± 0.0003		0.8107 ± 0.0011	300
—	10^6	—	0.1087 ± 0.0001	—	0.8097 ± 0.0003	8
			0.1093 ± 0.0001		0.8100 ± 0.0003	3000

Table 2: Solution of the bi-harmonic equation: the first line of each row contains the results for our algorithm, the second line contains the results for the Random Walk on rectangles.

Although a small numerical bias seems to appear, our algorithm provides results comparable with the method of random walk on rectangles, with an execution time much more smaller than the one given by this method (and also the one given by the random walk on squares, for which simulating a step takes less time, but where more steps are needed).

5.3 Estimation of rare events: computing hitting probabilities

We consider the simple problem: what is the probability $p(x)$ that starting from a point x in a domain D a Brownian motion reaches a part S of the boundary ∂D? It is well known that p is solution to the Dirichlet problem

$$\frac{1}{2}\triangle p(x) = 0 \text{ on } D \text{ and } p(x) = \begin{cases} 1 & \text{if } x \in S, \\ 0 & \text{if } x \in \partial D \setminus S. \end{cases} \tag{22}$$

We illustrate our method on the simple $2d$-domain D drawn in Figure 2 and we compute the value of p at the five points marked respectively by (a), (b), (c), (d) and (e) on Figure 2.

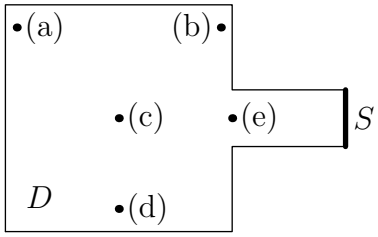

Figure 2: A simple domain D.

To set up our algorithm, we use 2 rectangles as in Figure 3, where the marked numbers are the probabilities we choose to reach each of the side. The exit time is drawn by using an exponential random variable of parameter one over the square of half the length of the rectangle in the direction perpendicular to the boundary the particle reaches. The exit position is uniform on each side.

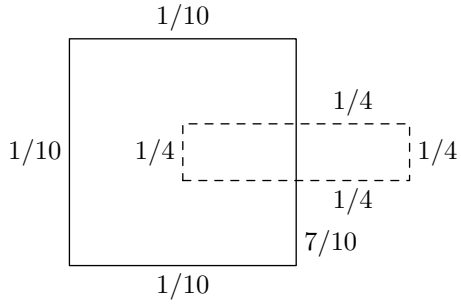

Figure 3: Decomposition of D into rectangles.

We perform 100.000 samples, and each computation takes around 1s on our computer. The values for p are given in Table 3. We perform a comparison with the value given by MATLAB/PDEtool, where (22) is solved using a finite element method, and with the method of random walk on rectangles [DL06] which is exact, up to the Monte Carlo error, for such a domain. In this case, with a sample of size n, the variance of the empirical mean is $p(x)(1-p(x))/n$.

We see that the results given by our method are very close to the one given by the finite elements methods. As one can expect, the random walk on rectangles (and then other methods that do not rely on importance sampling or variance reduction techniques) is not efficient to estimate the values of $p(x)$

Point	Import. Sampling	Finite Element	Walk on rect.
(a)	$3.32 \cdot 10^{-6}$	$3.39 \cdot 10^{-6}$	0.00
(b)	$2.31 \cdot 10^{-5}$	$2.23 \cdot 10^{-5}$	$1.00 \cdot 10^{-5}$
(c)	$1.70 \cdot 10^{-4}$	$1.77 \cdot 10^{-4}$	$1.90 \cdot 10^{-4}$
(d)	$4.43 \cdot 10^{-5}$	$4.64 \cdot 10^{-5}$	$3.00 \cdot 10^{-5}$
(e)	$2.79 \cdot 10^{-3}$	$2.81 \cdot 10^{-3}$	$2.36 \cdot 10^{-3}$

Table 3: Computation of $p(x)$ at the given points of D.

where they are of the same order as the standard deviation of the empirical mean.

In order to test the validity of our method for the simulation of rare events, we use the domain D' as in Figure 4.

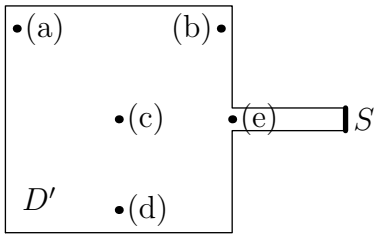

Figure 4: A simple domain D'.

The numerical results are reported in Table 4, where μ_n is the empirical average with $n = 100.000$ samples, and $\sigma_{50}(\mu_n)$ is the empirical standard deviation computed over 50 realizations of μ_n. We still get very good results, even while computing probabilities of order of magnitude 10^{-10}.

Point	μ_n	$\sigma_{50}(\mu_n)$	Finite Element
(a)	$1.00 \cdot 10^{-10}$	$2.3 \cdot 10^{-11}$	$1.15 \cdot 10^{-10}$
(b)	$7.67 \cdot 10^{-10}$	$1.6 \cdot 10^{-10}$	$8.13 \cdot 10^{-10}$
(c)	$5.19 \cdot 10^{-9}$	$1.0 \cdot 10^{-9}$	$6.61 \cdot 10^{-9}$
(d)	$1.31 \cdot 10^{-9}$	$2.8 \cdot 10^{-10}$	$1.73 \cdot 10^{-9}$
(e)	$2.27 \cdot 10^{-7}$	$4.9 \cdot 10^{-8}$	$2.29 \cdot 10^{-7}$

Table 4: Computation of $p(x)$ at the given points of D'.

5.4 Simulation of SDEs and estimation of PDE problems

In this section, we consider the 2-dimensional SDE

$$X_t = x + \int_0^t \sigma(X_s)\,\mathrm{d}B_s \text{ with } \sigma(x) = \begin{bmatrix} 1 & \frac{1}{2}\sin(x+y) \\ 0 & 1 \end{bmatrix} \tag{23}$$

which is driven by a 2-dimensional Brownian motion B. The process X is killed when it exits from the small domain D which is represented in Figure 5.

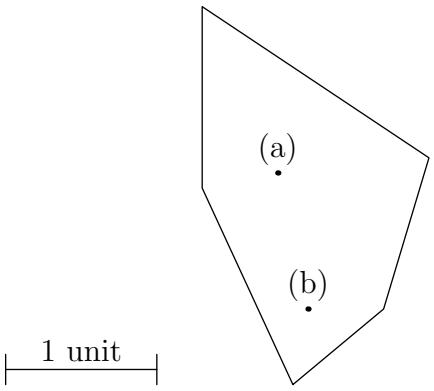

Figure 5: Domain D.

In order to simulate X, we use both either an Euler scheme with a time step of 0.0025 or a (possibly modified) random walk on squares with squares whose sides lengths are smaller than $2L$ with $L = 0.05$ (note that the time step of the Euler scheme corresponds to 0.05^2, which is close to the average exit time of the square $[0.1, 0.1]^2$). As the diffusion moves in a bounded domain, we use to deal with the boundary condition and apply the technique proposed in [CL02]: If the distance between the position of the particle and the boundary is smaller than $2L$, we choose the square so that one of its side is included in the part of the boundary if it is possible to do so.

When the Euler scheme is used, then simply stop the algorithm when the particle leaves the domain D. This is a crude way to proceed, and some refinements can be done (see [Gob00] for example). Note that the exit time is then over-estimated.

For the random walk on squares algorithm, we used tabulated values, and the algorithms is in average 5 times more time consuming than the Euler scheme.

In a first series of tests, we estimate $\mathbb{P}_x[\tau > T]$ for T large and the two starting points x represented in Figure 5. The results are given in Table 5.

The scheme MRW denotes the use of a modified random walk with the following strategy: when we succeed in constructing a square of side length smaller than $2L$ with one side included in the boundary, then we draw the exit side with probability $1\,\%$ for this side, and $0.33\,\%$ for the other sides. The scheme RW denotes the random walk on squares. The Euler is for the Euler scheme.

The parameter N corresponds to the number of samples. The confidence interval corresponds to $[\mu - 2\sqrt{\sigma}, \mu + 2\sqrt{\sigma}]$, where μ and σ are the estimated mean and variance of the quantity we compute. The quantities μ_w and σ_w are respectively an estimation of the mean and the variance of the weights: the closer from 1 and 0, the better.

The conclusion one can draw from this numerical study is that the Euler scheme fails when the probability to estimate is too small. The random walk (RW) and modified random walk (MRW) perform better. In our case, the MRW does not perform really better than the RW. Yet there have been no optimization between. The modified random walk is thus promising for evaluating small probabilities.

Scheme	N	$\mathbb{P}_x[\tau > T]$	Conf. interval	μ_w	σ_w
Case 1: $T = 4$, $x =$(a)					
MRW	10^6	$4.6 \cdot 10^{-5}$	$[3.2 \cdot 10^{-5}, 5.9 \cdot 10^{-5}]$	0.93	153.3
MRW	10^5	$3.9 \cdot 10^{-5}$	$[0.0, 7.9 \cdot 10^{-5}]$	0.93	47.8
RW	10^6	$12.2 \cdot 10^{-5}$	$[9.9 \cdot 10^{-5}, 14.4 \cdot 10^{-5}]$	—	—
RW	10^5	$14.2 \cdot 10^{-4}$	$[6 \cdot 10^{-5}, 21 \cdot 10^{-5}]$	—	—
Euler	10^6	0.0	—	—	—
Case 2: $T = 2$, $x =$(a)					
MRW	10^6	$5.1 \cdot 10^{-5}$	$[4.5 \cdot 10^{-5}, 7.7 \cdot 10^{-5}]$	0.93	153.3
MRW	10^5	$4.6 \cdot 10^{-5}$	$[0.3 \cdot 10^{-5}, 8.8 \cdot 10^{-5}]$	0.93	46.5
RW	10^6	$16.5 \cdot 10^{-5}$	$[13.9 \cdot 10^{-5}, 19.0 \cdot 10^{-5}]$	—	—
RW	10^5	$14 \cdot 10^{-5}$	$[6 \cdot 10^{-5}, 21 \cdot 10^{-5}]$	—	—
Euler	10^6	$2.9 \cdot 10^{-5}$	$[1.8 \cdot 10^{-5}, 4.0 \cdot 10^{-5}]$	—	—
Euler	10^5	$3.0 \cdot 10^{-5}$	$[0.5 \cdot 10^{-5}, 6.5 \cdot 10^{-5}]$	—	—
Case 3: $T = 4$, $x =$(b)					
MRW	10^6	$20 \cdot 10^{-6}$	$[11 \cdot 10^{-6}, 29 \cdot 10^{-6}]$	0.93	555.1
MRW	10^5	$5 \cdot 10^{-6}$	$[0.0, 19 \cdot 10^{-6}]$	0.99	234.8
RW	10^6	$57 \cdot 10^{-6}$	$[40 \cdot 10^{-6}, 72 \cdot 10^{-6}]$	—	—
RW	10^5	$80 \cdot 10^{-6}$	$[2.3 \cdot 10^{-5}, 13.7 \cdot 10^{-5}]$	—	—
Euler	10^6	0.0	—	—	—
Case 4: $T = 2$, $x =$(b)					
MRW	10^6	$3.8 \cdot 10^{-5}$	$[2.6 \cdot 10^{-5}, 5.1 \cdot 10^{-5}]$	0.96	554.1
MRW	10^5	$0.5 \cdot 10^{-5}$	$[0.0, 1.9 \cdot 10^{-5}]$	0.98	234.7
RW	10^6	$5.7 \cdot 10^{-5}$	$[4.2 \cdot 10^{-5}, 7.2 \cdot 10^{-5}]$	—	—
RW	10^5	$8.0 \cdot 10^{-5}$	$[2.3 \cdot 10^{-5}, 13.7 \cdot 10^{-5}]$	—	—
Euler	10^6	$1.9 \cdot 10^{-5}$	$[1.0 \cdot 10^{-5}, 2.8 \cdot 10^{-5}]$	—	—
Euler	10^5	$4 \cdot 10^{-5}$	$[0, 8 \cdot 10^{-5}]$	—	—

Table 5: Computing the probability that the diffusion is still in the domain at time T

A How to get densities for different situations?

We present in this section analytical expressions for the density in different cases.

Except in the case of a Brownian motion with drift and a Dirichlet boundary condition at one endpoint of $[-1, 1]$ and a Neumann boundary condition

at the other endpoint of $[-1,1]$, we obtain two expressions, one which follows from the use of the images method and the other from the spectral decomposition. From the numerical point of view, the spectral decomposition gives rise to series that converges very quickly for large times, while it is worth using the expressions given by the method of images if the time is small enough.

A.1 Brownian motion without drift

We are interested in this section in writing down some useful formulas for the calculations. We consider first the case of the standard one dimensional Brownian motion starting from $x \in [-1,1]$ which is killed or reflected when touching the boundaries -1 or 1. We shall write D for Dirichlet condition on the boundary and N for Neumann condition, which of course correspond to killing and respectively reflection. Furthermore we shall note, for example, $p_{DN}(t,x,y)$ for the density of the Brownian motion on $[-1,1]$ killed when touching -1 and reflected on 1, more precisely the order in the indices indicates the boundary condition in -1 and 1 respectively.

A.1.1 Reflected Brownian Motion on $[-1,1]$

Let $p_{NN}(t,x,y)$ denote the probability density function of a Brownian motion at time t, starting from x and reflected at -1 and 1. By using the method of image we get the following formula for the transition density:

$$p_{NN}(t,x,y) = \frac{1}{\sqrt{2\pi t}} \sum_{n=-\infty}^{\infty} \left[e^{-\frac{(x-y+4n)^2}{2t}} + e^{-\frac{(x+y+4n+2)^2}{2t}} \right].$$

The spectral representation of this density writes:

$$p_{NN}(t,x,y) = \frac{1}{2} + \sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2}{8}t} \cos\left(\frac{n\pi}{2}(x+1)\right) \cos\left(\frac{n\pi}{2}(y+1)\right).$$

These expressions may be found for example in [BCHSL92].

A.1.2 Killed Brownian Motion on $[-1,1]$

Let $p_{DD}(t,x,y)$ denote the probability density function of a Brownian motion at time t, starting from x and killed when it exits from the interval $[-1,1]$. That is

$$p_{DD}(t,x,y)dy = \mathbb{P}_x[B_t \in \mathrm{d}y; t < \tau_{DD}]$$

where $\tau_{DD} = \inf\{t \geq 0; B_t \notin [-1,1]\}$. Then, by the images' method we have:

$$p_{DD}(t,x,y) = \frac{1}{\sqrt{2\pi t}} \sum_{n=-\infty}^{\infty} \left[e^{-\frac{(x-y+4n)^2}{2t}} - e^{-\frac{(x+y+4n+2)^2}{2t}} \right].$$

For the law of the exit time we get:

$$\mathbb{P}_x[\tau_{DD} \in \mathrm{d}t] = \frac{1}{\sqrt{2\pi t^3}} \sum_{n=-\infty}^{\infty} (-1)^n (x+2n+1) e^{-\frac{(x+2n+1)^2}{2t}} \, \mathrm{d}t.$$

The spectral representation can be also written and yields:

$$p_{DD}(t,x,y) = \sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2}{8}t} \sin\left(\frac{n\pi}{2}(x+1)\right) \sin\left(\frac{n\pi}{2}(y+1)\right).$$

The law of the exit time is given by:

$$\mathbb{P}_x[\tau_{DD} \in \mathrm{d}t] = \frac{\pi}{2} \sum_{n=0}^{\infty} (-1)^n (2n+1) e^{-\frac{(2n+1)^2\pi^2}{8}t} \cos\left(\left(n+\frac{1}{2}\right)\pi x\right) \mathrm{d}t.$$

These expressions may be found for example in [BCHSL92] or in [MT99].

A.1.3 Mixed boundary conditions for the Brownian Motion on $[-1,1]$

We give here explicit solutions for the Brownian motion killed on -1 and reflected on 1. Let $p_{DN}(t,x,y)$ denote the probability density function of a Brownian motion at time t, starting from x and killed when it hits -1 and reflected on 1. Then, by the images' method,

$$p_{DN}(t,x,y) = \frac{1}{\sqrt{2\pi t}} \sum_{n=-\infty}^{\infty} (-1)^n \left[e^{-\frac{(x-y+4n)^2}{2t}} - e^{-\frac{(x+y+4n+2)^2}{2t}} \right].$$

Let us denote also by τ_{DN} the killing time for the Brownian motion on $[-1,1[$ killed on -1 and reflected on 1. Hence,

$$\mathbb{P}_x[\tau_{DN} \in \mathrm{d}t] \;\; = \frac{1}{\sqrt{2\pi t^3}} \sum_{n=-\infty}^{\infty} (-1)^n (x+4n+1) e^{-\frac{(x+4n+1)^2}{2t}} \, \mathrm{d}t.$$

The spectral representation can be also written and yields:

$$p_{DN}(t,x,y) = \sum_{n=0}^{\infty} e^{-\frac{(2n+1)^2\pi^2}{32}t} \sin\left(\frac{(2n+1)\pi}{4}(x+1)\right) \sin\left(\frac{(2n+1)\pi}{4}(y+1)\right).$$

Then we get from the spectral representation the law of this exit time:

$$\mathbb{P}_x[\tau_{DN} \in \mathrm{d}t] = \frac{\pi}{8}\sum_{n=0}^{\infty}(2n+1)e^{-\frac{(2n+1)^2\pi^2}{32}t}\sin\left(\frac{(2n+1)\pi}{4}(x+1)\right)\mathrm{d}t.$$

The dual situation (reflection on -1 and absorption on 1) can be obtained easily by the transformation

$$p_{ND}(t,x,y) = p_{DN}(t,-x,y).$$

These expressions may be found for example in [BCHSL92].

A.2 Brownian motion with drift μ

As in the previous part of the appendix we consider here the case of the Brownian motion on the interval $[-1,1]$ which is killed or reflected on -1 and 1. If we note by $p_{\cdot\cdot}^{L,\mu}(t,x,y)$ the law of the process with drift μ and living on $[-L,L]$ and $p_{\cdot\cdot}^{\mu}(t,x,y)$ the corresponding law on $[-1,1]$ then, by the properties of the Brownian motion we have:

$$p_{\cdot\cdot}^{L,\mu}(t,x,y) = \frac{1}{L}p_{\cdot\cdot}^{\mu L}\left(\frac{t}{L^2},\frac{x}{L},\frac{y}{L}\right),$$

where the dots in the indices can take the value D for a Dirichlet condition or N for a Neumann condition, as previously noted.

A.2.1 Brownian motion with drift μ reflected on $[-1,1]$

We keep the same notations as before. The use of images' method gives the following representation of the density:

$$\begin{aligned}p_{NN}^{\mu}(t,x,y) = {} & \frac{2\mu e^{2\mu y}}{e^{2\mu}-e^{-2\mu}} + \frac{1}{\sqrt{2\pi t}}\sum_{n=-\infty}^{\infty} e^{4\mu n}e^{-\frac{(x-y+\mu t+4n)^2}{2t}} \\ & + \frac{1}{\sqrt{2\pi t}}\sum_{n=-\infty}^{\infty} e^{-2\mu x}e^{-\mu(4n+2)}e^{-\frac{(x+y-\mu t+4n+2)^2}{2t}} \\ & - \mu e^{2\mu y}\sum_{n=-\infty}^{\infty} e^{\mu(4n+2)}\operatorname{erfc}\left(\frac{x+y+\mu t+4n+2}{\sqrt{2t}}\right).\end{aligned}$$

This formula can be obtained also from the results in D. Veestraeten [Vee05].

By the spectral method (see for example [Lin05]), we have after some calculations:

$$p^{\mu}_{NN}(t,x,y) = \frac{2\mu e^{2\mu y}}{e^{2\mu}-e^{-2\mu}} + e^{\mu(y-x)-\frac{\mu^2}{2}t}\sum_{n=1}^{\infty}\frac{e^{-\frac{n^2\pi^2}{8}t}}{\mu^2+\frac{n^2\pi^2}{4}} \times\left[\frac{\pi n}{2}\cos\left(\frac{\pi n}{2}(x+1)\right)+\mu\sin\left(\frac{\pi n}{2}(x+1)\right)\right] \times\left[\frac{\pi n}{2}\cos\left(\frac{\pi n}{2}(y+1)\right)+\mu\sin\left(\frac{\pi n}{2}(y+1)\right)\right].$$

A.2.2 Brownian motion with drift μ on $[-1,1]$ killed at the boundary

We keep the same notations as before. By using classical properties of the Brownian motion and the results from Milstein and Tretyakov [MT99] we have the following transformation:

$$p^{\mu}_{DD}(t,x,y) = e^{\mu(y-x)-\frac{\mu^2 t}{2}}p_{DD}(t,x,y).$$

Then, by the images' method,

$$p^{\mu}_{DD}(t,x,y) = e^{\mu(y-x)-\frac{\mu^2 t}{2}}\frac{1}{\sqrt{2\pi t}}\sum_{n=-\infty}^{\infty}\left[e^{-\frac{(x-y+4n)^2}{2t}}-e^{-\frac{(x+y+4n+2)^2}{2t}}\right].$$

We write down both distribution and density for the exit time. The distribution writes:

$$\mathbb{P}_x[\tau^{\mu}_{DD}<t] = 1-\frac{1}{2}\sum_{n=-\infty}^{\infty}e^{4\mu n}\left[\mathrm{erfc}\left(\frac{x+\mu t+4n-1}{\sqrt{2t}}\right)-\mathrm{erfc}\left(\frac{x+\mu t+4n+1}{\sqrt{2t}}\right)\right] +\frac{1}{2}\sum_{n=-\infty}^{\infty}e^{-(2\mu x+\mu(4n+2))}\left[\mathrm{erfc}\left(\frac{x-\mu t+4n+1}{\sqrt{2t}}\right)-\mathrm{erfc}\left(\frac{x-\mu t+4n+3}{\sqrt{2t}}\right)\right].$$

While for the density we obtain:

$$\mathbb{P}_x[\tau^{\mu}_{DD}\in \mathrm{d}t] = \frac{e^{-\mu x-\frac{\mu^2 t}{2}}}{\sqrt{2\pi t^3}}\sum_{n=-\infty}^{\infty}\left[e^{-\mu}(x+4n+1)e^{-\frac{(x+4n+1)^2}{2t}}- -e^{\mu}(x+4n-1)e^{-\frac{(x+4n-1)^2}{2t}}\right].$$

The spectral representation can be also written and yields:

$$p^{\mu}_{DD}(t,x,y) = e^{\mu(y-x)-\frac{\mu^2 t}{2}}\sum_{n=1}^{\infty}e^{-\frac{n^2\pi^2}{8}t}\sin\left(\tfrac{n\pi}{2}(x+1)\right)\sin\left(\tfrac{n\pi}{2}(y+1)\right).$$

The distribution of the exit time is given by:

$$\begin{aligned}
&\mathbb{P}_x[\tau_{DD}^{\mu} < t] \\
&\quad = 1 - e^{-\mu x - \frac{\mu^2 t}{2}} \sum_{n=1}^{\infty} (e^{-\mu} - (-1)^n e^{\mu}) \tfrac{2n\pi}{4\mu^2 + n^2\pi^2} e^{-\frac{n^2\pi^2}{8} t} \sin\left(\tfrac{n\pi}{2}(x+1)\right) \\
&\quad = 1 - e^{-\mu x - \frac{\mu^2 t}{2}} (e^{-\mu} - e^{\mu}) \sum_{n=1}^{\infty} (-1)^n \tfrac{n\pi}{\mu^2 + n^2\pi^2} e^{-\frac{n^2\pi^2}{2} t} \sin(n\pi x) \\
&-e^{-\mu x - \frac{\mu^2 t}{2}} (e^{-\mu} + e^{\mu}) \sum_{n=0}^{\infty} (-1)^n \tfrac{2(2n+1)\pi}{4\mu^2 + (2n+1)^2\pi^2} e^{-\frac{(2n+1)^2\pi^2}{8} t} \cos\left(\tfrac{(2n+1)\pi}{2} x\right)
\end{aligned}$$

and

$$\mathbb{P}_x[\tau_{DD}^{\mu} \in \mathrm{d}t] = e^{-\mu x - \frac{\mu^2 t}{2}} \sum_{n=1}^{\infty} \tfrac{n\pi}{4} (e^{-\mu} - (-1)^n e^{\mu}) e^{-\frac{n^2\pi^2}{8} t} \sin\left(\tfrac{n\pi}{2}(x+1)\right) \mathrm{d}t.$$

In a more detailed expression we can write this on the form:

$$\begin{aligned}
\mathbb{P}_x[\tau_{DD}^{\mu} \in \mathrm{d}t] &= e^{-\mu x - \frac{\mu^2 t}{2}} (e^{-\mu} - e^{\mu}) \sum_{n=1}^{\infty} (-1)^n \tfrac{n\pi}{2} e^{-\frac{n^2\pi^2}{2} t} \sin(n\pi x) \\
&+e^{-\mu x - \frac{\mu^2 t}{2}} (e^{-\mu} + e^{\mu}) \sum_{n=0}^{\infty} (-1)^n \tfrac{(2n+1)\pi}{4} e^{-\frac{(2n+1)^2\pi^2}{8} t} \cos\left(\tfrac{(2n+1)\pi}{2} x\right) \mathrm{d}t.
\end{aligned}$$

These expressions may be found for example in [BCHSL92] or in [MT99].

A.2.3 Mixed boundary condition for the Brownian Motion on $[-1, 1]$ with drift μ

The aim is to express some explicit solutions for the Brownian motion killed on -1 and reflected on 1. We are solving the following eigenvalue problem:

$$\begin{cases} \frac{1}{2}\varphi''(x) + \mu\varphi'(x) = \lambda\varphi(x) \\ \varphi(-1) = 0 \\ \varphi'(1) = 0. \end{cases}$$

We can remark first that if φ_λ is a eigenfunction for the eigenvalue λ in the preceding PDE then λ is negative.

We associate to this problem the corresponding second degree equation and note $\Delta = \mu^2 + 2\lambda$. After a detailed calculus with respect to the sign of Δ we can express the countable set of eigenfunctions and eigenvalues with respect to the possible values of μ. There are three different situations, expressed in the Table 6 (see the book [Pin98] for example). The density $p_{DN}(t, x, y)$ is obtained by using the spectral expansion

μ	λ	φ_λ
$\mu < \frac{1}{2}$	$\lambda \leq -\frac{\mu^2}{2}$, $\tan(2\sqrt{-\mu^2-2\lambda}) = \frac{\sqrt{-\mu^2-2\lambda}}{\mu}$	$\frac{e^{-\mu x}}{\sqrt{2\left(1-\frac{\cos^2(2\sqrt{-\mu^2-2\lambda})}{2\mu}\right)}} \sin(\sqrt{-\mu^2-2\lambda}(x+1))$
$\mu = \frac{1}{2}$	$-\frac{1}{8}$	$\frac{\sqrt{3}}{4} e^{-\frac{x}{2}}(x+1)$
	$\lambda < -\frac{1}{8}$, $\tan\left(2\sqrt{\left(\frac{1}{4}+2\lambda\right)}\right) = 2\sqrt{\left(\frac{1}{4}+2\lambda\right)}$	$\frac{e^{-\frac{x}{2}}}{\sqrt{2}\left\lvert\sin\left(2\sqrt{\frac{1}{4}+2\lambda}\right)\right\rvert} \sin\left(\sqrt{\frac{1}{4}+2\lambda}(1+x)\right)$
$\mu > \frac{1}{2}$	$\lambda \geq -\frac{\mu^2}{2}$, $\tanh(2\sqrt{\mu^2+2\lambda}) = \frac{\sqrt{\mu^2+2\lambda}}{\mu}$	$\frac{e^{-\mu x}}{\sqrt{\frac{2\cosh^2(2\sqrt{\mu^2+2\lambda})}{\mu}-1}} \sinh(\sqrt{\mu^2+2\lambda}(x+1))$
	$\lambda \leq -\frac{\mu^2}{2}$, $\tan(2\sqrt{-\mu^2-2\lambda}) = \frac{\sqrt{-\mu^2-2\lambda}}{\mu}$	$\frac{e^{-\mu x}}{\sqrt{2\left(1-\frac{\cos^2(2\sqrt{-\mu^2-2\lambda})}{2\mu}\right)}} \sin(\sqrt{-\mu^2-2\lambda}(x+1))$

Table 6: Eigenvalues and eigenfunctions for the Dirichlet/Neumann problem with a constant transport term μ.

$p_{DN}(t,x,y) = \sum_{k\geq 0} \exp^{\lambda_k t} \varphi_{\lambda_k}(x)\varphi_{\lambda_k}(y)$, where $\cdots \leq \lambda_2 \leq \lambda_1 < \lambda_0$. The density $q_{DN}(t,x)$ of the exit time is also expressed by

$$\mathbb{P}_x[\tau_{DN} \in \mathrm{d}t]/\,\mathrm{d}t = -\sum_{k\geq 0} \lambda_k e^{\lambda_k t} \phi_{\lambda_k}(x) \int_{-1}^{1} \phi_{\lambda_k}(y)\,\mathrm{d}y.$$

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