Uncertain Darcy's problem and the stochastic particle transport

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1 Expected exit time from a domain

We aim to estimate the exit time of a particle driven by a deterministic transport field and a stochastic diffusion from a domain $D \subset \mathbb{R}^d$. Given a vector $W(t)$ of m independent Brownian motions and two functions $f\colon \mathbb{R}^d \to \mathbb{R}^d, g\colon \mathbb{R}^d \to \mathbb{R}^{d\times m}$, we consider the following stochastic differential equation (SDE)

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases} \tag{1}$$

The problem is completed with two different types of boundary conditions, namely

i. *killing boundaries*: if the particle exits D the process is stopped,

ii. *reflecting boundaries*: the particle trajectory is reflected normally inside D when it touches the boundary ∂D.

Our aim is to estimate numerically the first exit time of the solution $X(t)$ from D, *i.e.*, the quantity

$$\tau = \min\{\min\{t\colon X(t) \notin D\}, T\}. \tag{2}$$

Let us remark that the parameter τ is meaningful only if there exists a portion of the boundary $\Gamma_k \subset \partial D$ that is endowed with killing boundary conditions. Otherwise, the process $X(t)$ will stay in D for the whole time interval, giving as a result $\tau = T$ for each realisation of $X(t)$. Another quantity of interest is defined as follows

$$\phi = \phi(T, X_0, F) = \mathbb{1}_{\{\tau<T\}} F(X(T)), \tag{3}$$

where $F\colon \mathbb{R}^d \to \mathbb{R}$ is a smooth function. An interesting choice of F could be the function mapping every x of $\mathbb{R}^d$ to the value 1. In this case, the expecation of ϕ is equal to the probability for $X(t)$ to exit the domain before the final time T. Let us choose the notation $F = 1$ in this case, getting

$$\Phi(T, X_0) = \mathbb{E}(\phi(T, X_0, 1)) = \Pr(\tau < T | X(0) = X_0) \tag{4}$$

In the case of general f, g and for a d-dimensional SDE, there is no closed form for τ and ϕ. Therefore, we approximate the value of τ by means of two numerical schemes, briefly presented in the following.

1.1 Numerical Methods

1.1.1 Discrete Euler-Maruyama

Given $N \in \mathbb{N}$ let us define a partition of $[0,T]$ as $P_h = \{t_i\}_{i=0}^N, t_i = ih, h = T/N$. The Discrete Euler-Maruyama method (DEM) for problem (1) is defined as follows

$$\begin{cases} X_h^d(t_{i+1}) = f(X(t_i))h + g(X(t_i))(W(t_{i+1}) - W(t_i)), \\ X_h^d(0) = X_0. \end{cases} \tag{5}$$

The exit time τ is approximated with the quantity τ_h^d defined as

$$\tau_h^d = \min\{\min\{t_i \colon X_h^d(t_i) \notin D\}, T\}. \tag{6}$$

We approximate analogously ϕ as

$$\phi_h^d = \mathbb{1}_{\{\tau_h^d < T\}} F(X_h^d(T)). \tag{7}$$

Let us state two results concerning the weak error of this method.

Proposition 1.1 *Under appropriate assumptions of smoothness of $f, g, D, \partial D, F$,*

$$|\mathbb{E}(\tau_h^d) - \mathbb{E}(\tau)| = O(\sqrt{h}). \tag{8}$$

Proposition 1.2 *Under approprate assumptions of smoothness of $f, g, D, \partial D, F$,*

$$|\mathbb{E}(\phi_h^d) - \mathbb{E}(\phi)| = O(\sqrt{h}). \tag{9}$$

An discussion of result 1.1 can be found in [5], its proof in [3]. A proof of 1.2 can be found in [1].

1.1.2 Continuous Euler-Maruyama.

Let us consider the partition P_h of $[0,T]$ as above. The Continuous Euler-Maruyama (CEM) method is defined as

$$\begin{cases} X_h^c(t) = f(X(t_i))(t - t_i) + g(X(t_i))(W(t) - W(t_i)), \quad t_i < t \le t_{i+1}, \\ X_h^c(0) = X_0. \end{cases} \tag{10}$$

Let us remark that in case the particle does not exit the domain, $X_h^c(t_i) = X_h^d(t_i)$ for all $t_i \in P_h$. It is possible to compute the probability that a particle has exited the domain at a time t between two consecutive timesteps t_i, t_{i+1} when D is an half-space with the following formula [2]

$$\mathbb{P}(\exists t \in [t_i, t_{i+1}] \quad X_h^d(t) \notin D | X_h^d(t_i) = x_i, X_h^d(t_{i+1}) = x_{i+1}) = p(x_i, x_{i+1}, h), \tag{11}$$

with $p(x_i, x_{i+1}, h)$ given by

$$p(x_i, x_{i+1}, h) = \exp\Big(-2 \frac{[n \cdot (x_i - z_i)][n \cdot (x_{i+1} - z_i)]}{hn \cdot (gg^T(x_i)n)} \Big), \tag{12}$$

where z_i is the projection of x_i on ∂D and n is the normal to ∂D in z_i. At each timestep t_{i+1} we compute the probability $p(x_i, x_{i+1}, h)$, and then simulate a variable U distributed uniformly in the interval $[0,1]$, thus obtaining a realization u. Hence, we counclude that

Algorithm 1: Continuous Euler-Maruyama

```
for t_i ∈ P_h do
    Compute X(t_{i+1}) with one step of DEM ;
    if X(t_{i+1}) ∉ D then
        τ_h^c = t_{i+1} ;
        φ_h^c = F(X_h^c(t_{i+1}) ;
        return;
    else
        compute p = p(x_i, x_{i+1}, h) ;
        simulate u ~ Unif(0, 1) ;
        if u < p then
            τ_h^c = t_{i+1} ;
            φ_h^c = F(X_h^c(t_{i+1}) ;
            return;
        end
    end
end
```

the particle has left the domain for a time t in (t_i, t_{i+1}) if u is smaller than p. Therefore, we approximate the exit time as

$$\tau_h^c = \min\{T, \min\{t_i = hi \colon X_h(t_i) \notin D\}, \min\{t_i = hi \colon u < p(x_{i-1}, x_i, h)\}\}, \qquad (13)$$

In the same way as in DEM, we can approximate ϕ as

$$\phi_h^c = \mathbb{1}_{\{\tau_h^c < T\}} F(X_h^c(T)). \qquad (14)$$

We show the pseudocode for the implementation of CEM in Algorithm 1.
The weak error of this method has been studied exhaustively in previous work.

Proposition 1.3 *Under appropriate smoothness assumptions,*

$$|\mathbb{E}(\phi_h^c) - \mathbb{E}(\phi)| = O(h). \qquad (15)$$

A proof of result 1.3 can be found in [2].

1.1.3 Reflecting boundaries

The reflecting boundaries are treated in the same way for both DEM and CEM. Let us denote by Γ_k and Γ_r the killing and reflecting subsets of ∂D, *i.e.*

$$\Gamma_r \cup \Gamma_k = \partial D, \quad \Gamma_r \cap \Gamma_k = \emptyset \qquad (16)$$

In case the particle approaches Γ_k the exit is treated as above. If for a timestep of $t_i \in P_h$, $X(t_i)$ is not in D and has crossed Γ_r at a time $t_{i-1} < t < t_i$, we update the solution to be the normal reflection inside D of $X(t_i)$.

1.2 A PDE approach

It is possible to express the mean exit time and the probability of exit from a domain in terms of the solution of partial differential equations (PDE's). Let us denote by Γ_k, Γ_r the killing and reflecting subsets of ∂D. We consider then the expectation of the exit time from the domain D for a trajectory that at $t = 0$ is at position x, *i.e.*,

$$\bar{\tau}(x) = \mathbb{E}(\tau | X(0) = x). \tag{17}$$

Let us define the operator $\mathcal{L}$ induced by (1) acts on a function $u\colon \mathbb{R}^d \to \mathbb{R}$ as follows

$$\mathcal{L}u = f \cdot \nabla u + \frac{1}{2} g g^T : \nabla \nabla u, \tag{18}$$

where the : operator between two matrices A, B in $\mathbb{R}^{d \times d}$ is defined as follows

$$A : B = \sum_{i,j=1}^{d} \{A\}_{ij} \{B\}_{ij} = \mathrm{tr}(A^T B). \tag{19}$$

The following result allows computing the mean exit time as the solution of an appropriate PDE.

Proposition 1.4 *Let $\mathcal{L}$ be the differential operator defined as* (18). *Then, if Γ_k and Γ_r are respectively the killing and reflecting subsets of ∂D, such that $\Gamma_k \cup \Gamma_r = \partial D, \Gamma_k \cap \Gamma_r = \emptyset$, the mean exit time $\bar{\tau}(x)$ for the solution $X(t)$ of* (1) *with $X_0 = x$ is the solution of the following boundary value problem*

$$\begin{cases} \mathcal{L}\bar{\tau}(x) = -1, & \textit{in } D, \\ \bar{\tau}(x) = 0, & \textit{on } \Gamma_k, \\ \nabla \bar{\tau}(x) \cdot n = 0, & \textit{on } \Gamma_r, \end{cases} \tag{20}$$

where n is the normal to Γ_r.

Further analytical treatement of the mean exit time can be found in [6, 7].
We now consider the probability of exit from D for a solution $X(t)$ that is equal to x for $t = s < T$. This probability is the solution of a boundary value problem.

Proposition 1.5 *Let $\mathcal{L}$ be the differential operator defined as* (18). *Then, if Γ_k and Γ_r are respectively the killing and reflecting subsets of ∂D, such that $\Gamma_k \cup \Gamma_r = \partial D, \Gamma_k \cap \Gamma_r = \emptyset$*

$$\Pr(\tau < T | X(s) = x) = \Phi(x, s, T) \tag{21}$$

where $\Phi(x, t, T)$ is the solution of the following backwards PDE

$$\begin{cases} \frac{\partial}{\partial t} \Phi(x, t, T) + \mathcal{L}\Phi(x, t, T) = 0 & \textit{in } D, s \le t < T, \\ \Phi(x, t, T) = 1 & \textit{on } \Gamma_k, s \le t < T, \\ \nabla \Phi(x, t, T) \cdot n = 0, & \textit{on } \Gamma_r, s \le t < T, \\ \Phi(x, T, T) = 0 & \textit{in } D, \end{cases} \tag{22}$$

where n is the normal to Γ_r.

The proof in case $\Gamma_k = \partial D$ of this result can be found in [8]. Further treatment in case of mixed boundary conditions and the closed form of the solution for some particular geometries of $D \subset \mathbb{R}^2$ can be found in [4]. It is therefore possible to approximate $\bar{\tau}$ and Φ by means of classical methods for solving PDE's numerically, such as finite differences or the Finite Elements Method.

1.3 One-Dimensional Case

We consider problem (1) in case $d = 1$. Given $f, g\colon \mathbb{R} \to \mathbb{R}$, an interval $D = [l, r]$ and a Brownian motion $W(t)$, let us consider the following one dimensional SDE

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases} \tag{23}$$

In this case, the boundary of D consists of the two points $\{l, r\}$. In order for the problem of the determination of τ to be meaningful, at least one of the two points should be endowed with a killing boundary condition.

1.3.1 Analytical expression of the mean exit time

In this simple frame, it is possible to deduce an analytical solution $\bar{\tau}$ of (20). Let us consider the boundary condition at $x = l$ fixed as *killing* and vary the boundary condition at $x = r$. Since the scope is deducing the exit time of a particle from D, this assumption is plausible. In this frame, it is possible to rewrite (20) as

$$\begin{cases} f(x)\bar{\tau}'(x) + \frac{1}{2}g^2(x)\bar{\tau}''(x) = -1, & l < x < r, \\ \bar{\tau}(l) = 0, & \\ \bar{\tau}(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{killing}, \\ \bar{\tau}'(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{reflecting}. \end{cases} \tag{24}$$

It is possible to show [6, 7] that $\bar{\tau}$ is in the one-dimensional case given by

$$\bar{\tau}(x) = -2\int_l^x \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy + c_1 \int_l^x \exp(-\psi(y))dy + c_2, \tag{25}$$

where the function ψ is defined as

$$\psi(x) = \int_l^x \frac{2f(y)}{g^2(y)} dy, \tag{26}$$

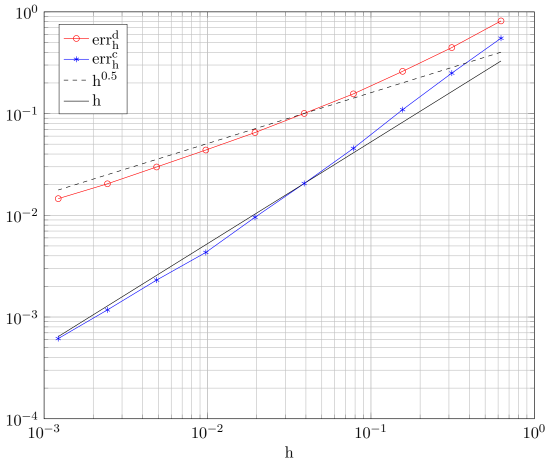
and the constants $c_1, c_2 \in \mathbb{R}$ depend on the boundary conditions as follows

$$\begin{aligned} c_1 &= 2\frac{\int_l^r \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy}{\int_l^r \exp(-\psi(y))dy}, \text{ if for } x = r \text{ the boundary is } \textit{killing}, \\ c_1 &= 2\int_l^r \frac{\exp(-\psi(y))}{g(y)^2} dy, \text{ if for } x = r \text{ the boundary is } \textit{reflecting}, \\ c_2 &= 0. \end{aligned} \tag{27}$$

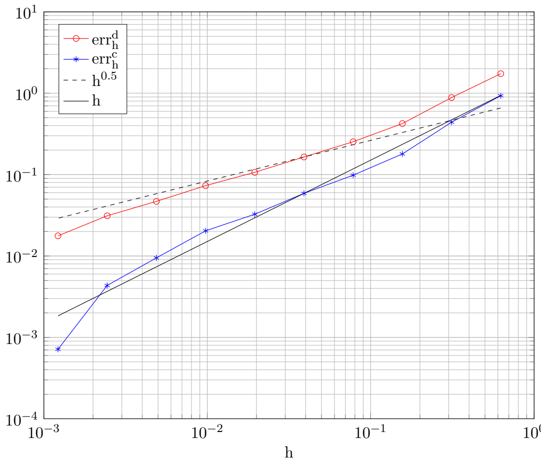
Let us remark that in case $f = -V'$ for some smooth function V and $g = \sigma \in \mathbb{R}$, the expression of ψ semplifies to

$$\psi(x) = 2\frac{V(l) - V(x)}{\sigma^2}. \tag{28}$$

The value for the expected exit time given by (25) will be used as a reference for verifying the order of convergence of the numerical methods.



(a) Killing boundary in $x = 1$



(b) Reflecting boundary in $x = 1$

Figure 1: Orders of convergence for DEM and CEM in the one-dimensional case.

1.3.2 Numerical experiments

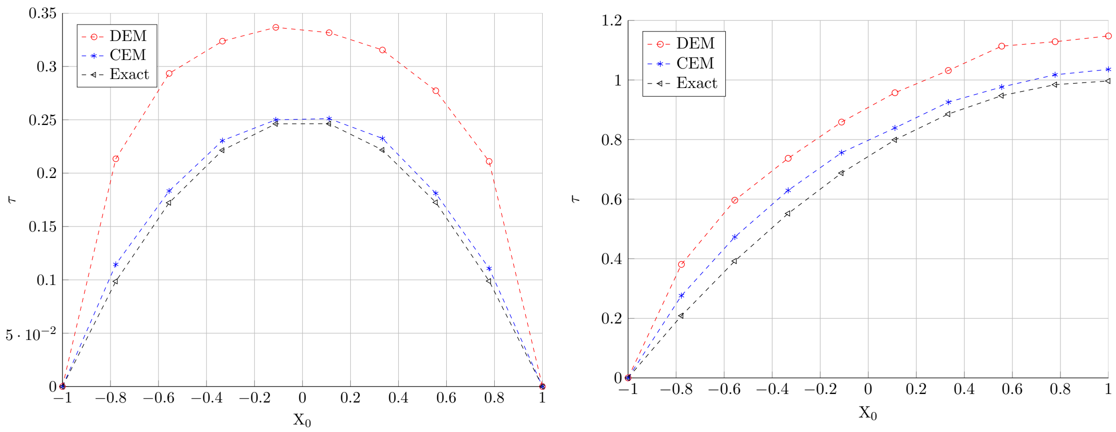
Smooth case. We consider as a domain for (23) the interval $D = [-1, 1]$, final time $T = 5$ and the following functions

$$\begin{aligned} &f(x) = -V'(x), \text{ where } V(x) = 0.1(8x^4 - 8x^2 + x + 2), \\ &g(x) = \sigma = 3. \end{aligned} \tag{29}$$

We approximate the value of τ with a Montecarlo simulation of τ_h^d and τ_h^c computed as in (6) and (13) from the solutions provided by DEM and CEM respectively. In order to verify the order of convergence of the methods, we let N vary in the set $2^i, i = 3, \dots, 12$ and we fix the number of trajectories M to 10000. In this way, the error caused by the Montecarlo estimation should not spoil the order of convergence. In Figure 1 we show the errors obtained fixing $X_0 = 0$ in both the cases of killing and reflecting boundary conditions in $x = 1$. Moreover, in Figure 2 we show an approximation of τ obtained with the two methods with $h = T/128$ and $M = 1000$ for a set of 10 initial values equispaced along D. It is possible to remark that computing the probability of exit between two consecutive timesteps as in (12) allows correcting the overestimation of τ obtained simply using DEM. We want to estimate the computational time for both the method. We consider $M = 10000$, killing boundary conditions and $N = 2^i, i = 3, \dots, 12$. It is possible to remark in Figure 3 that the computational time required by CEM is higher than for DEM if the same value of h is employed. On the other hand, fixing the error, CEM is faster than DEM in this case.

Rough case. We consider the same domain D as above, $T = 5$ and $g = \sigma = 3$. We consider V to be piecewise linear, so that $f = -dV$ is piecewise constant. In particular, we choose the following form for V

$$V = 0.1 \begin{cases} -2x - 1 & x < -0.5, \\ 4x + 2 & -0.5 \leq x < 0, \\ -2x + 2 & 0 \leq x < 0.5, \\ 4x - 1 & x \geq 0.5. \end{cases} \tag{30}$$



(a) Killing boundary in $x = 1$

(b) Reflecting boundary in $x = 1$

Figure 2: Approximation of τ for the discrete and continuous EM method in the one-dimensional case.

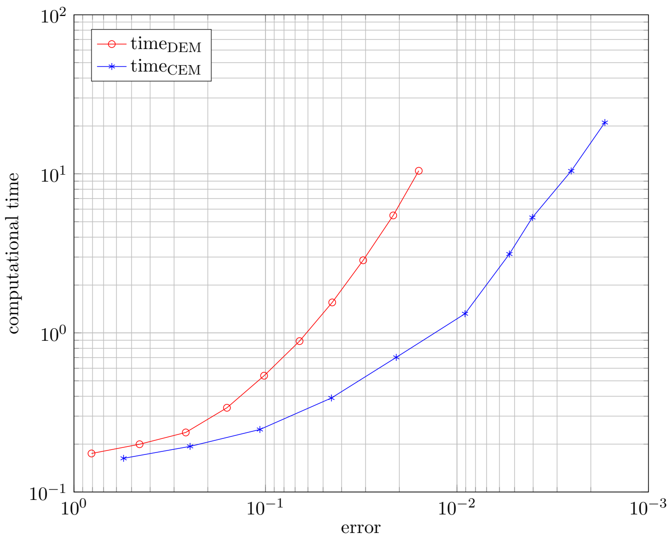


Figure 3: error vs work plot for DEM and CEM.

This is a linear interpolation of the function V we used in the smooth case above in the points $\{-1, -0.5, 0, 0.5, 1\}$ (Figure 4). This case is of particular interest, since if the function f is the result of a numerical method on a PDE, it could not be smooth as in the previous case. We perform DEM and CEM with the same parameters as before, *i.e.*, $M = 10000, N = 2^i, i = 3, \ldots, 12$. In Figure 5 it is possible to remark that the rate of convergence of DEM is unvaried with respect to the previous case. The CEM method experiences a slight decrease in the order of convergence with respect to the smooth case.

1.4 Two-dimensional case

We are interested in estimating the exit time of a particle from a domain $D \subset \mathbb{R}^2$. Given $W(t)$ a vector of two independent Brownian motions, we consider the equation (1). In this case, $f\colon \mathbb{R}^2 \to \mathbb{R}^2, g\colon \mathbb{R}^2 \to \mathbb{R}^{2\times 2}$. We compute the mean exit time and the exit probability using DEM and CEM and compare results with the numerical solution of the PDE's presented in 1.2.

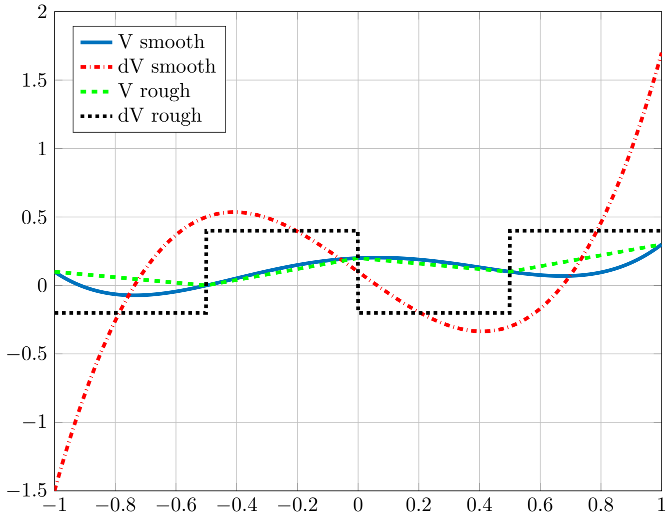


Figure 4: V and dV employed in the numerical experiments in both the smooth and rough cases.

1.4.1 Numerical experiments - Estimation of τ

Killing boundary conditions. We consider a simple case of (1) in $D = [-1, 1] \times [-1, 1]$, where

$$f = 0 \in R^2, \; g = \sigma I \in R^{2\times 2}, \sigma \in \mathbb{R}.$$

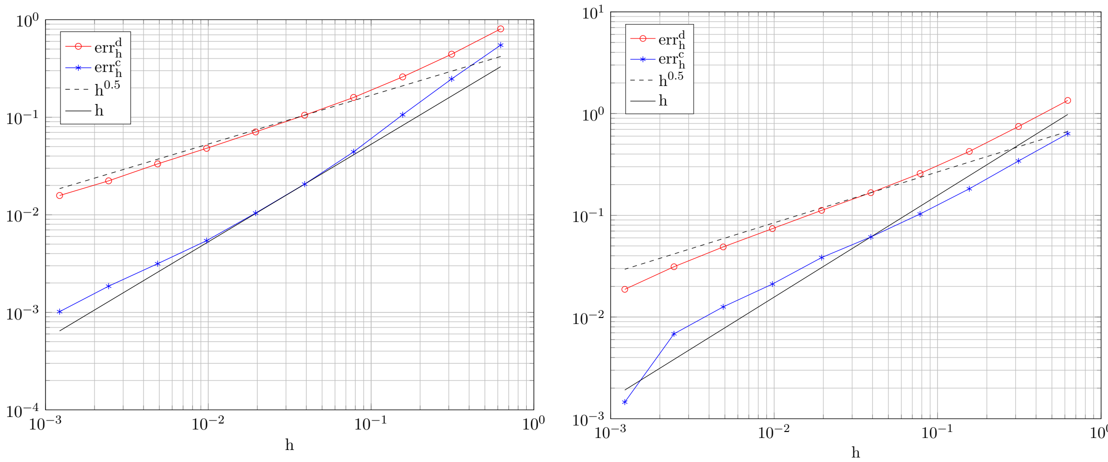
Moreover, we consider ∂D to be a killing boundary. The solution in this case is a Brownian motion. In this case, the partial differential equation (20) reduces to

$$\begin{cases} -\sigma^2 \Delta \bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \partial D. \end{cases} \tag{31}$$

This is the Poisson equation, hence it is possible to solve it numerically with the Finite Elements Method or the finite differences avoiding a high computational cost. We use the Finite Elements Method adopting a regular mesh with equal constant spacing in the x and y directions, obtaining a solution as in Figure 6b. In order to verify the orders of convergence of DEM and CEM, we set $T = 3$, $\sigma = 1$, $X_0 = (0, 0)^T$, with $M = 10000$ and $N = 2^i, i = 3, \ldots, 9$. We then compare the Montecarlo estimation we obtain with the value of $\bar{\tau}$ in $(0, 0)$, obtained by interpolation on the Finite Elements solution. The orders of convergence for this numerical experiment are shown in Figure 6a. The results confirm the theoretical orders of convergence for DEM and CEM, with an average order of 0.55 for DEM and 0.93 for CEM, which corrects to 0.98 if the last point is not taken into account.

Mixed boundary conditions. We consider the same problem as above with mixed killing and reflecting boundary conditions. f and g are the same as above, so the SDE model does not change, but we consider the two left and right boundaries of D, defined by $x = \pm 1$, to be reflecting. We denote this portion of the boundary as Γ_r, and the rest as Γ_k. In this case, the equation for $\bar{\tau}$ becomes

$$\begin{cases} -\sigma^2 \Delta \bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \Gamma_k, \\ \partial \bar{\tau} \cdot n = 0, & \text{on } \Gamma_r. \end{cases} \tag{32}$$



(a) Killing boundary in $x = 1$

(b) Reflecting boundary in $x = 1$

Figure 5: Orders of convergence for DEM and CEM in the one-dimensional case with f piecewise constant.

The solution of this equation is shown in Figure 7b. We compute the expectation of τ with DEM and CEM with the same parameters as above. The results (Figure 7a), show that the theoretical orders of convergence are not spoilt by this choice of boundary conditions. The mean order for DEM in this case is 0.55, while for CEM it is 1.15.

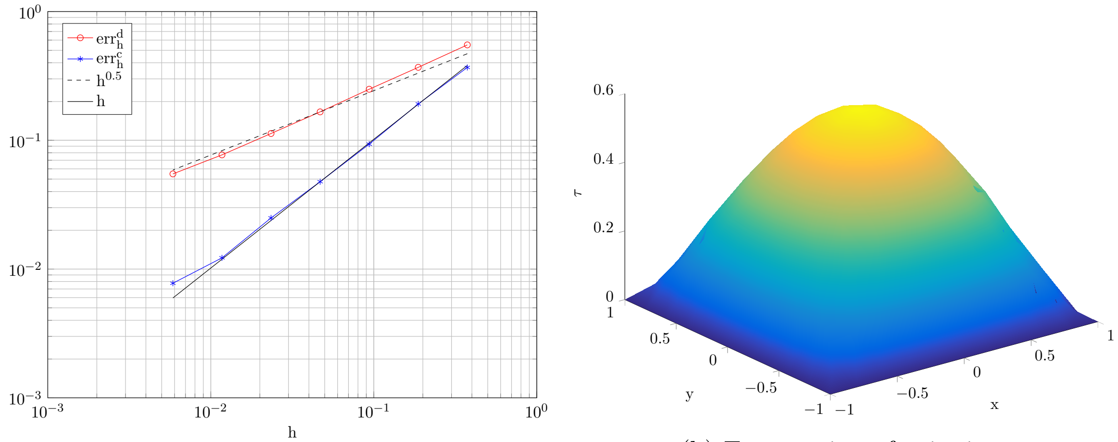
1.4.2 Numerical experiments - Estimation of Φ

Killing boundary conditions. We consider the same simple case as in section 1.4.1 We consider ∂D to be a killing boundary. The solution of (1) is in this case a Brownian motion. In this case, the partial differential equation (22) reduces to

$$\begin{cases} \frac{\partial}{\partial t}\Phi(x,t,T) + \frac{1}{2}\sigma^2\Delta\Phi(x,t,T) = 0, & \text{in } D, 0 \le t < T, \\ \Phi(x,t,T) = 1, & \text{on } \partial D, 0 \le t < T, \\ \Phi(x,T,T) = 0, & \text{in } D. \end{cases} \tag{33}$$

We solve this problem numerically with the Finite Elements Method as for (32). The solution at $t = 0$ is shown in Figure 8b. We verify the orders of convergence of DEM and CEM setting $X_0 = (0,0)^T, \sigma = 1, T = 1$. We consider $M = 100000$ trajectories and $N = 2^i, i = 0, \dots, 5$. We then compare the Montecarlo estimation with the value of Φ in $(0,0)$, obtained by interpolation on the Finite Elements solution. The orders of convergence for this numerical experiment are shown in Figure 8a. The theoretical orders of convergence are confirmed in this case as well, with an average order of 0.43 for DEM and 1.19 for CEM.

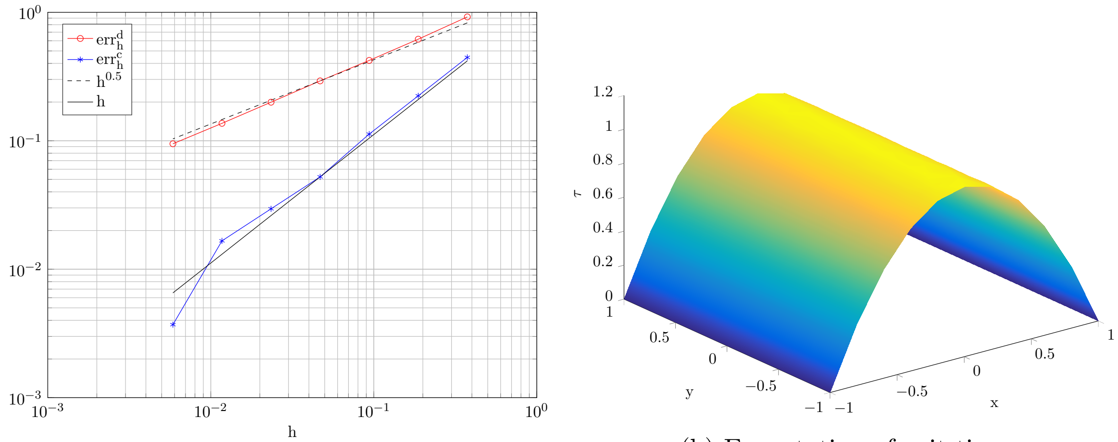
Mixed boundary conditions. We consider the same values for the parameters, the time integration and the Montecarlo estimation as in the pure killing case. In this case, we set the boundary conditions to be reflecting on the subset of the boundary of D defined by $x = \pm 1$ and killing for the other boundaries.Therefore, in this case the exit probability Φ



(a) Convergence of CEM and DEM.

(b) Expectation of exit time.

Figure 6: Summary of the results for τ in the two-dimensional case with pure killing boundary conditions.



(a) Convergence of CEM and DEM.

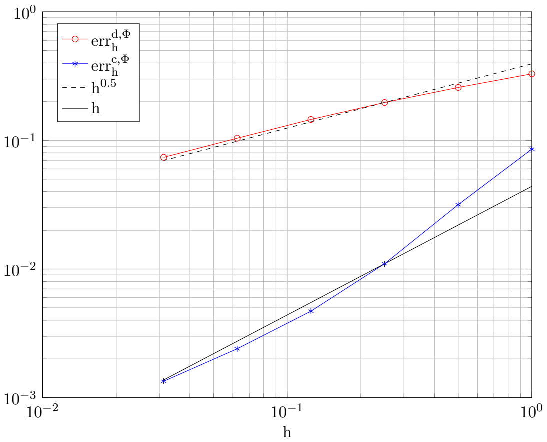
(b) Expectation of exit time.

Figure 7: Summary of the results for τ in the two-dimensional case with mixed boundary conditions.

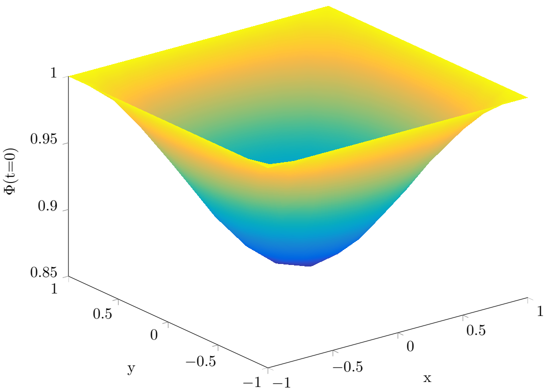
is the solution of the folllowing PDE

$$\begin{cases} \frac{\partial}{\partial t}\Phi(x,t,T) + \frac{1}{2}\sigma^2\Delta\Phi(x,t,T) = 0, & \text{in } D, 0 \le t < T, \\ \Phi(x,t,T) = 1, & \text{on } \Gamma_k, 0 \le t < T, \\ \nabla\Phi(x,t,T) \cdot n = 0, & \text{on } \Gamma_r, 0 \le t < T, \\ \Phi(x,T,T) = 0, & \text{in } D. \end{cases} \tag{34}$$

The solution of this equation computed with Finite Elements is shown in Figure 9b. The convergence results for DEM and CEM are shown in Figure 9a. The mean orders in this case are 0.37 for DEM and 0.87 for CEM, which is less than the prediction given by theoretical results. This decrease in the convergence rate is remarkable for small values of h. This could mean that the error caused by the Finite Element approximation of the solution of (34) is not negligible with respect to the error of CEM.

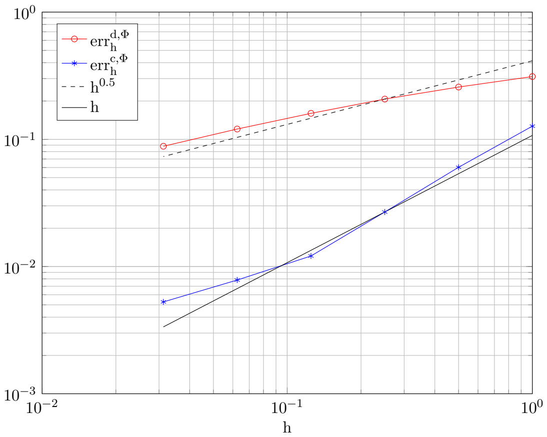


(a) Convergence of CEM and DEM.

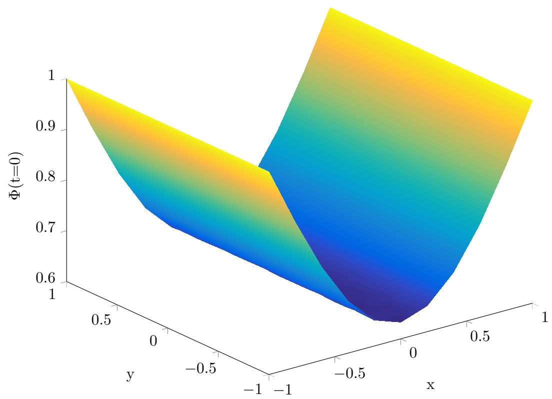


(b) Probability of exit.

Figure 8: Summary of the results for Φ in the two-dimensional case with pure killing boundary conditions.



(a) Convergence of CEM and DEM.



(b) Probability of exit.

Figure 9: Summary of the results for Φ in the two-dimensional case with mixed boundary conditions.

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