

# Uncertain Darcy's problem and the stochastic particle transport

Giacomo Garegnani

Supervisors: Dr. Sebastian Krumscheid and Prof. Fabio Nobile

## Contents

<b>1</b>	<b>Expected exit time from a domain</b>	<b>2</b>
1.1	Numerical Methods . . . . .	2
1.1.1	Discrete Euler-Maruyama . . . . .	2
1.1.2	Continuous Euler-Maruyama. . . . .	3
1.1.3	Reflecting boundaries . . . . .	4
1.1.4	An adaptive procedure . . . . .	4
1.2	A PDE approach . . . . .	5
1.3	One-Dimensional Case . . . . .	6
1.3.1	Analytical expression of the mean exit time . . . . .	6
1.3.2	Numerical experiments - Estimation of $\tau$ . . . . .	7
1.3.3	Numerical approximation of $\Phi$ with the PDE approach . . . . .	8
1.3.4	Numerical experiments - Estimation of $\Phi$ . . . . .	10
1.4	Two-dimensional case . . . . .	11
1.4.1	Numerical experiments - Estimation of $\tau$ . . . . .	11
1.4.2	Numerical experiments - Estimation of $\Phi$ . . . . .	13
1.4.3	Numerical experiments - Adaptivity . . . . .	14
<b>2</b>	<b>The uncertain Darcy problem</b>	<b>14</b>
2.1	Problem statement . . . . .	15
2.2	Finite Elements solution of the Darcy problem . . . . .	15
2.3	Solution of the SDE . . . . .	16
2.4	Summary . . . . .	18
2.5	Theoretical issues . . . . .	18
2.6	Numerical Experiment - Grid refinements . . . . .	20

# 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  $f: \mathbb{R}^d \rightarrow \mathbb{R}^d, g: \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$ , we consider the following stochastic differential equation (SDE)

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

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  $\partial D$ .

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

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

Let us remark that the parameter  $\tau$  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

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

where  $F: \mathbb{R}^d \rightarrow \mathbb{R}$  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 expectation of  $\phi$  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

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

In the case of general  $f, g$  and for a  $d$ -dimensional SDE, there is no closed form for  $\tau$  and  $\phi$ . Therefore, we approximate the value of  $\tau$  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

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

The exit time  $\tau$  is approximated with the quantity  $\tau_h^d$  defined as

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

We approximate analogously  $\phi$  as

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

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

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

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

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

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

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

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

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]

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

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

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

where  $z_i$  is the projection of  $x_i$  on  $\partial D$  and  $n$  is the normal to  $\partial D$  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 conclude that 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

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

In the same way as in DEM, we can approximate  $\phi$  as

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

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,*

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

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

**Algorithm 1:** Continuous Euler-Maruyama

```

for  $t_i \in P_h$  do
   $X(t_{i+1}) = f(X(t_i))h + g(X(t_i))(W(t_{i+1}) - W(t_i))$  ;
  if  $X(t_{i+1}) \notin D$  then
     $\tau_h^c = t_{i+1}$  ;
     $\phi_h^c = F(X_h^c(t_{i+1}))$  ;
    return;
  else
    compute  $p = p(x_i, x_{i+1}, h)$  ;
    simulate  $u \sim \text{Unif}(0, 1)$  ;
    if  $u < p$  then
       $\tau_h^c = t_{i+1}$  ;
       $\phi_h^c = F(X_h^c(t_{i+1}))$  ;
      return;
    end
  end
end

```

**1.1.3 Reflecting boundaries**

The reflecting boundaries are treated in the same way for both DEM and CEM. Let us denote by  $\Gamma_k$  and  $\Gamma_r$  the killing and reflecting subsets of  $\partial D$ , *i.e.*

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

In case the particle approaches  $\Gamma_k$  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  $\Gamma_r$  at a time  $t_{i-1} < t < t_i$ , we update the solution to be the normal reflection inside  $D$  of  $X(t_i)$ .

**1.1.4 An adaptive procedure**

Let us consider the function  $g$  in (1) to be fixed to a real constant  $\sigma$ . The numerical methods we presented can be completed with an adaptive procedure for the step size  $h$ . In this frame, adaptivity is performed with respect to the position of the numerical solution  $X_h(t_i)$ , *i.e.*, the step size is reduced if the solution is near to the boundary of the domain  $D$ . If we denote by  $d_i$  the distance between  $X_h(t_i)$  and its normal projection on  $\partial D$ , by  $l \in \mathbb{N}$  a fixed parameter and by  $h_0$  a maximum bound for  $h$ , the step size is chosen using the following formula

$$h = \max \left\{ 2^{-2l} h_0, \min \left\{ 2^{-l} h_0, \left( \frac{d}{(l+3)\sigma} \right)^2 \right\} \right\}. \quad (17)$$

This formula is equivalent to dividing the domain  $D$  in three zones, in particular

- an interior zone where  $h = h_{int} = 2^{-l} h_0$ ,
- a boundary zone where  $h = h_{bound} = 2^{-2l} h_0$ ,
- an intermediate zone where  $h = \frac{d^2}{(l+3)\sigma^2}$ .

Since the loss of 0.5 in the weak order of convergence of Euler-Maruyama is due to the non-detected exits from the domain  $D$ , refining the step size only near to the boundary could lead to an error equal to the one obtained using  $h_{bound}$  on the whole domain.

## 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  $\Gamma_k, \Gamma_r$  the killing and reflecting subsets of  $\partial D$ . 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.*,

$$\bar{\tau}(x) = \mathbb{E}(\tau | X(0) = x). \quad (18)$$

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

$$\mathcal{L}u = f \cdot \nabla u + \frac{1}{2} g g^T : \nabla \nabla u, \quad (19)$$

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

$$A : B = \sum_{i,j=1}^d \{A\}_{ij} \{B\}_{ij} = \text{tr}(A^T B). \quad (20)$$

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 (19). Then, if  $\Gamma_k$  and  $\Gamma_r$  are respectively the killing and reflecting subsets of  $\partial D$ , 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*

$$\begin{cases} \mathcal{L}\bar{\tau}(x) = -1, & \text{in } D, \\ \bar{\tau}(x) = 0, & \text{on } \Gamma_k, \\ \nabla \bar{\tau}(x) \cdot n = 0, & \text{on } \Gamma_r, \end{cases} \quad (21)$$

where  $n$  is the normal to  $\Gamma_r$ .

Further analytical treatment of the mean exit time can be found in [6, 8].

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 (19). Then, if  $\Gamma_k$  and  $\Gamma_r$  are respectively the killing and reflecting subsets of  $\partial D$ , such that  $\Gamma_k \cup \Gamma_r = \partial D, \Gamma_k \cap \Gamma_r = \emptyset$*

$$\Pr(\tau < T | X(s) = x) = \Phi(x, s, T) \quad (22)$$

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

$$\begin{cases} \frac{\partial}{\partial t} \Phi(x, t, T) + \mathcal{L}\Phi(x, t, T) = 0 & \text{in } D, s \leq t < T, \\ \Phi(x, t, T) = 1 & \text{on } \Gamma_k, s \leq t \leq T, \\ \nabla \Phi(x, t, T) \cdot n = 0, & \text{on } \Gamma_r, s \leq t \leq T, \\ \Phi(x, T, T) = 0 & \text{in } D, \end{cases} \quad (23)$$

where  $n$  is the normal to  $\Gamma_r$ .

The proof in case  $\Gamma_k = \partial D$  of this result can be found in [9]. 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  $\Phi$  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  $f, g: \mathbb{R} \rightarrow \mathbb{R}$ , an interval  $D = [l, r]$  and a Brownian motion  $W(t)$ , let us consider the following one dimensional SDE

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases} \quad (24)$$

In this case, the boundary of  $D$  consists of the two points  $\{l, r\}$ . In order for the problem of the determination of  $\tau$  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 (21). 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 (21) as

$$\begin{cases} f(x)\bar{\tau}'(x) + \frac{1}{2}g^2(x)\bar{\tau}''(x) = -1, & l < x < r, \\ \bar{\tau}(l) = 0, \\ \bar{\tau}(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{killing}, \\ \bar{\tau}'(r) = 0, & \text{if for } x = r \text{ the boundary is } \textit{reflecting}. \end{cases} \quad (25)$$

It is possible to show [6, 8] that  $\bar{\tau}$  is in the one-dimensional case given by

$$\bar{\tau}(x) = -2 \int_l^x \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy + c_1 \int_l^x \exp(-\psi(y)) dy + c_2, \quad (26)$$

where the function  $\psi$  is defined as

$$\psi(x) = \int_l^x \frac{2f(y)}{g^2(y)} dy, \quad (27)$$

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

$$\begin{aligned} c_1 &= 2 \frac{\int_l^r \exp(-\psi(z)) \int_l^z \frac{\exp(\psi(y))}{g^2(y)} dy}{\int_l^r \exp(-\psi(y)) dy}, & \text{if for } x = r \text{ the boundary is } \textit{killing}, \\ c_1 &= 2 \int_l^r \frac{\exp(-\psi(y))}{g(y)^2} dy, & \text{if for } x = r \text{ the boundary is } \textit{reflecting}, \\ c_2 &= 0. \end{aligned} \quad (28)$$

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

$$\psi(x) = 2 \frac{V(l) - V(x)}{\sigma^2}. \quad (29)$$

The value for the expected exit time given by (26) will be used as a reference for verifying the order of convergence of the numerical methods.

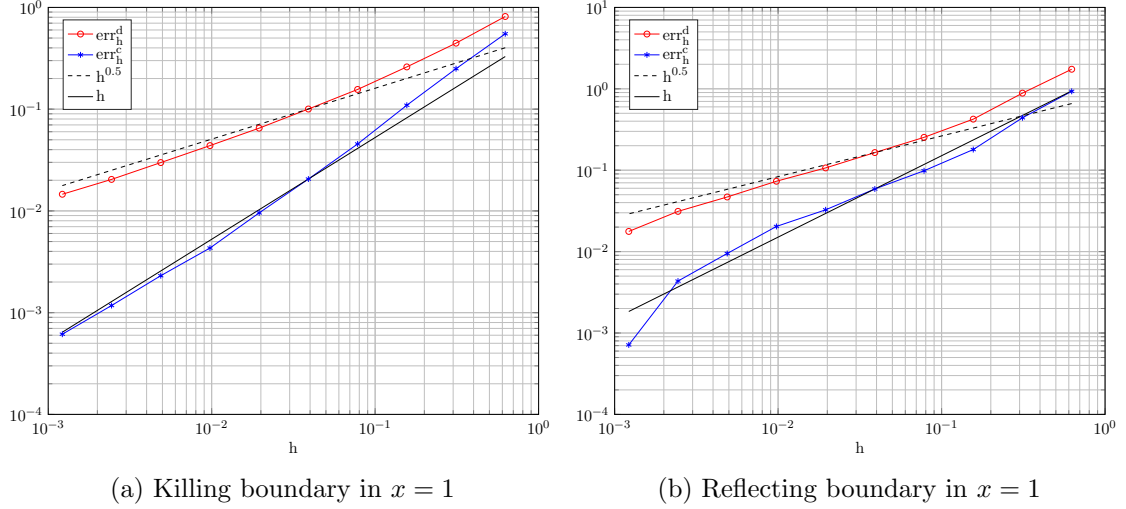


Figure 1: Approximation of  $\tau$ . Orders of convergence for DEM and CEM in the one-dimensional case.

### 1.3.2 Numerical experiments - Estimation of $\tau$

**Smooth case.** We consider as a domain for (24) the interval  $D = [-1, 1]$ , final time  $T = 5$  and the following functions

$$\begin{aligned} f(x) &= -V'(x), \text{ where } V(x) = 0.1(8x^4 - 8x^2 + x + 2), \\ g(x) &= \sigma = 3. \end{aligned} \quad (30)$$

We approximate the value of  $\tau$  with a Montecarlo simulation of  $\tau_h^d$  and  $\tau_h^c$  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  $\tau$  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  $\tau$  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  $V$

$$V = 0.1 \begin{cases} -2x - 1, & x < -0.5, \\ 4x + 2, & -0.5 \leq x < 0, \\ -2x + 2, & 0 \leq x < 0.5, \\ 4x - 1, & x \geq 0.5. \end{cases} \quad (31)$$

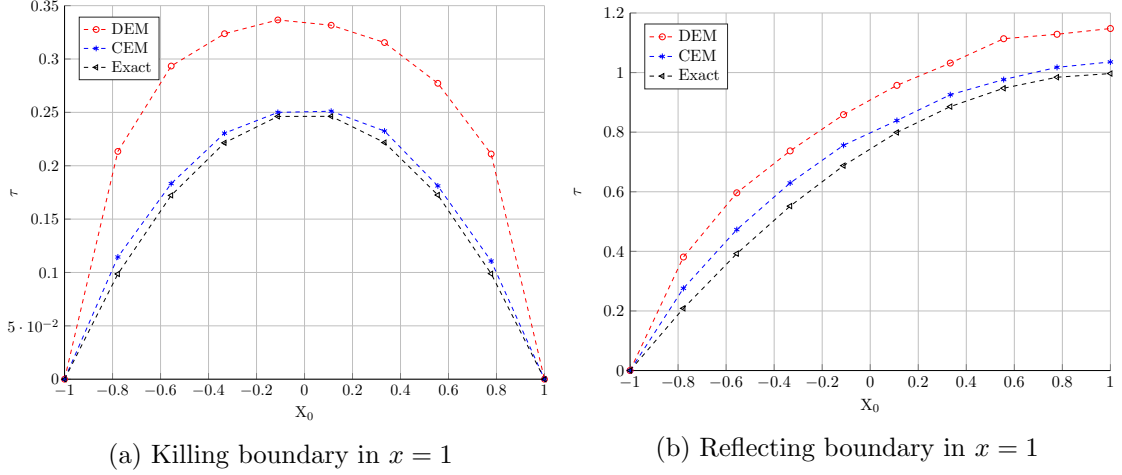


Figure 2: Approximation of  $\tau$  as a function of the initial value  $X_0$ .

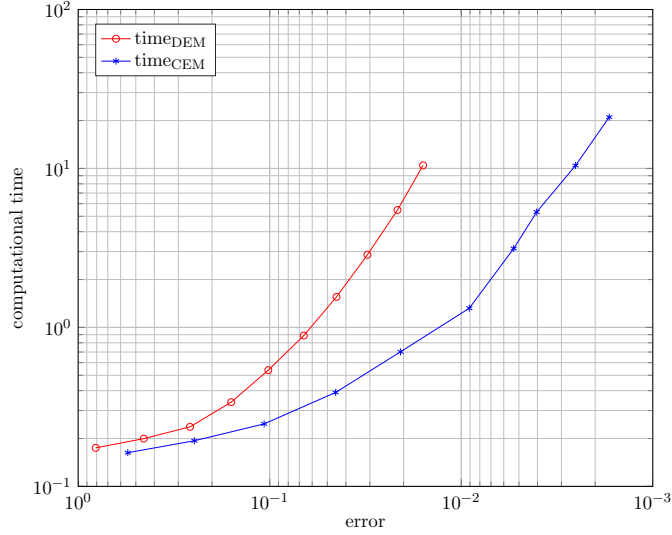


Figure 3: error vs work plot for DEM and CEM.

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.*,  $M = 10000, N = 2^i, i = 3, \dots, 12$ . 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.

### 1.3.3 Numerical approximation of $\Phi$ with the PDE approach

Let us consider  $D$  as the interval  $[l, r]$ , the boundary condition in  $l$  to be fixed to killing and in  $r$  to be either killing or reflecting. In this case and for  $f$  independent of  $t$  and



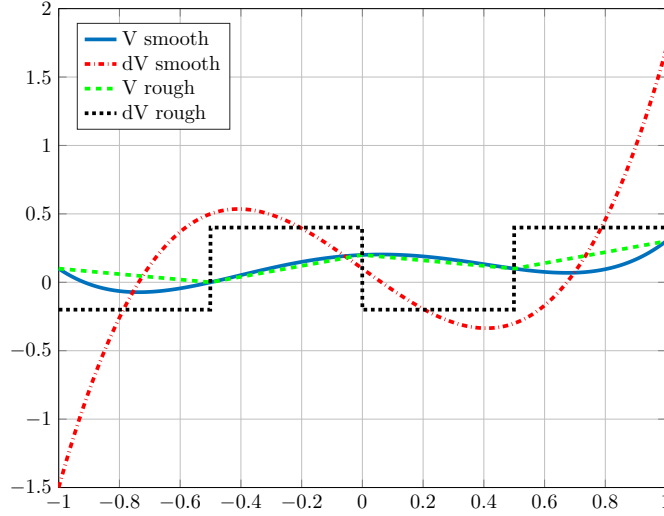


Figure 4:  $V$  and  $dV$  employed in the numerical experiments in both the smooth and rough cases.

$g = \sigma \in \mathbb{R}$  (23) can be written as the following initial value PDE

$$\left\{ \begin{array}{l} -\frac{\partial}{\partial t}\Phi(t, x) + f\frac{\partial}{\partial x}\Phi(t, x) + \frac{1}{2}\sigma^2\frac{\partial^2}{\partial x^2}\Phi(t, x) = 0, \quad l < x < r \\ \Phi(t, l) = 1, \\ \Phi(t, r) = 1, \quad \text{if for } x = r \text{ the boundary is } \textit{killing} \\ \frac{\partial}{\partial x}\Phi(t, r) = 0, \quad \text{if for } x = r \text{ the boundary is } \textit{reflecting} \\ \Phi(0, x) = 0. \end{array} \right. \quad (32)$$

This equation can be solved, *e.g.*, using finite differences. We employ the theta method for solving (32). Let us consider the case in which  $r$  is a killing boundary, *i.e.*, the PDE is endowed with Dirichlet boundary conditions. Given a step size  $\Delta_t$  for time integration and an uniform grid  $x_i = l + i\Delta_x, i = 0, \dots, N+1, x_{N+1} = r$ , at each timestep  $k$  one has to find the solution of the linear system

$$(I - \Delta_t\theta A)u^{k+1} = (I + \Delta_t(1 - \theta)A)u^k + hF, \quad 0 \leq \theta \leq 1, \quad (33)$$

where  $I$  is the identity matrix of  $\mathbb{R}^{N \times N}$ . The matrix  $A$  of  $\mathbb{R}^{N \times N}$  and the vector  $F$  of  $\mathbb{R}^N$  define the space discretization and the boundary conditions and are defined by

$$A = \frac{1}{2\Delta_x} \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \gamma_1 & \alpha_2 & \beta_2 & \\ & \ddots & \ddots & \ddots \end{pmatrix}, \quad F = \frac{1}{2\Delta_x} (F_1 \cdots F_N)^T \quad (34)$$

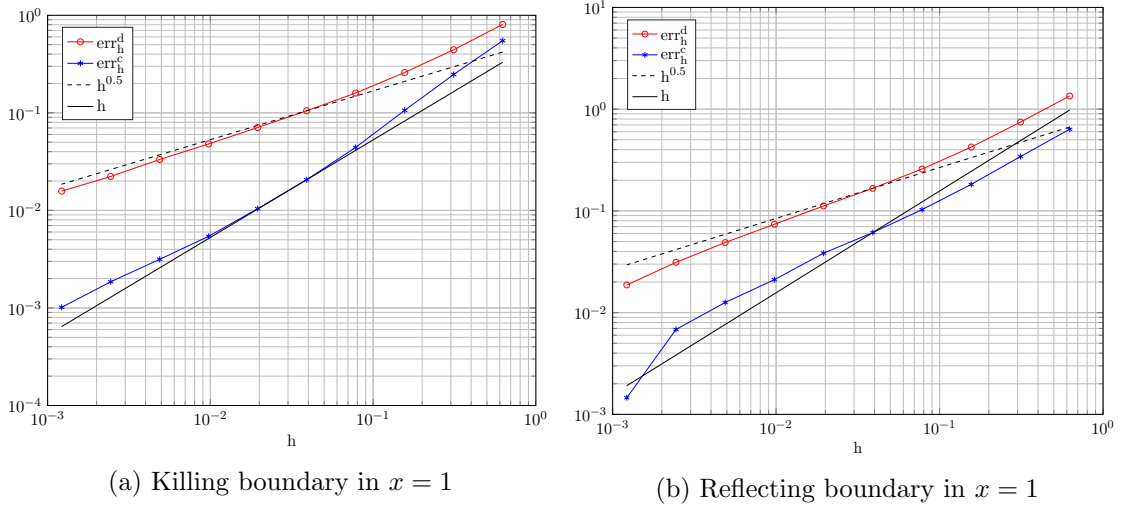


Figure 5: Approximation of  $\tau$ . Orders of convergence for DEM and CEM in the one-dimensional case with  $f$  piecewise constant.

and the coefficients are given by

$$\begin{aligned}
 \alpha_i &= -\frac{2\sigma^2}{\Delta_x}, \quad i = 1, \dots, N, \\
 \beta_i &= \frac{\sigma^2}{\Delta_x} + f(x_i), \quad i = 1, \dots, N-1, \\
 \gamma_i &= \frac{\sigma^2}{\Delta_x} - f(x_{i+1}), \quad i = 1, \dots, N-1, \\
 F_1 &= \frac{\sigma^2}{\Delta_x} - f(x_1), \\
 F_N &= \frac{\sigma^2}{\Delta_x} - f(x_{N-1}).
 \end{aligned} \tag{35}$$

The case of reflecting boundary condition in  $x = r$  is similar and affects only the computation of the matrix  $A$  and the vector  $F$ . In particular, we introduce a *ghost node* at position  $x = r + \Delta_x$ , compute the derivative using a centrate approximation and impose that it is equal to 0, which leads to the condition that the value in the node in  $x = r$  is equal to the value in  $x = r - \Delta_x$ . Since the matrix defining the system (33) is tridiagonal, one can choose  $\Delta_t, \Delta_x$  to be small and obtain a precise solution of (32) in a reasonable computational time. In the following, we will compare the values given by Montecarlo simulations using DEM and CEM with the solution of the theta method with  $\theta = 0.5$ .

#### 1.3.4 Numerical experiments - Estimation of $\Phi$

**Smooth case.** We consider (24) with  $D = [-1, 1]$ , the final time  $T = 0.5$  and we define

$$\begin{aligned}
 f(x) &= -V'(x), \quad \text{where } V(x) = 8x^4 - 8x^2 + x + 2, \\
 g(x) &= \sigma = 2.
 \end{aligned} \tag{36}$$

In order to approximate  $\Phi$ , we perform a Montecarlo simulation using both DEM and CEM, with  $M = 6 \cdot 10^5$  trajectories in order to kill the statistical error. We consider the number of timesteps for the time integration to be  $N = 2^i, i = 5, \dots, 12$ . Numerical results

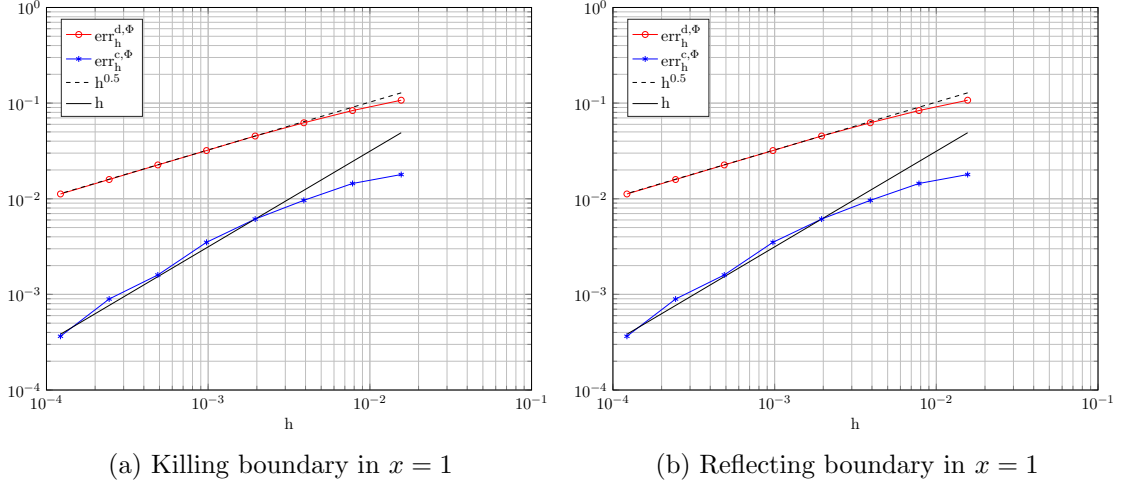


Figure 6: Approximation of  $\Phi$ . Orders of convergence of DEM and CEM in the one-dimensional case.

(Figure 6a) confirm that the weak error for DEM is of order 0.5, while for CEM the order of convergence is 1.

## 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,  $f: \mathbb{R}^2 \rightarrow \mathbb{R}^2, g: \mathbb{R}^2 \rightarrow \mathbb{R}^{2 \times 2}$ . 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.

### 1.4.1 Numerical experiments - Estimation of $\tau$

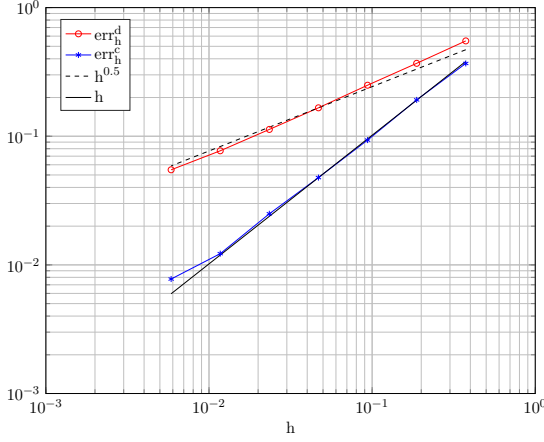
**Killing boundary conditions.** We consider a simple case of (1) in  $D = [-1, 1] \times [-1, 1]$ , where

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

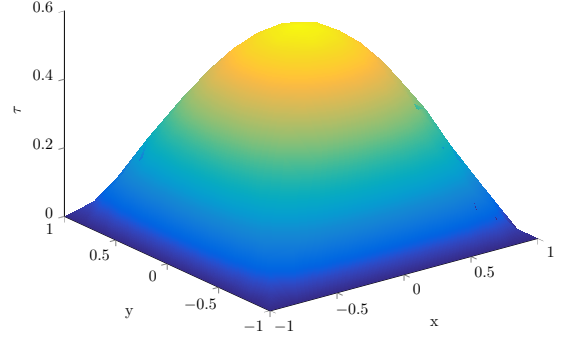
Moreover, we consider  $\partial D$  to be a killing boundary. The solution in this case is a Brownian motion. In this case, the partial differential equation (21) reduces to

$$\begin{cases} -\sigma^2 \Delta \bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \partial D. \end{cases} \quad (37)$$

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 7b. 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  $N = 2^i, i = 3, \dots, 9$ . 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 7a. 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.

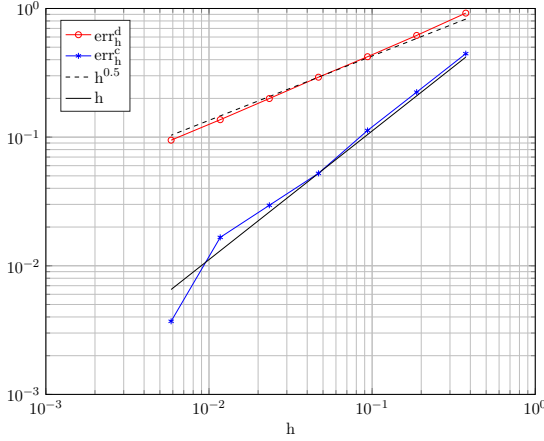


(a) Convergence of CEM and DEM.

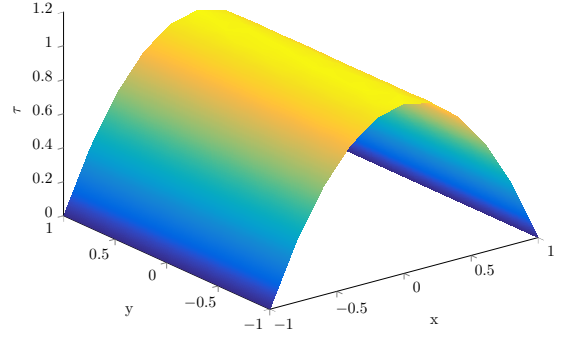


(b) Expectation of exit time.

Figure 7: Summary of the results for  $\tau$  in the two-dimensional case with pure killing boundary conditions.



(a) Convergence of CEM and DEM.



(b) Expectation of exit time.

Figure 8: Summary of the results for  $\tau$  in the two-dimensional case with mixed boundary conditions.

**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  $\Gamma_r$ , and the rest as  $\Gamma_k$ . In this case, the equation for  $\bar{\tau}$  becomes

$$\begin{cases} -\sigma^2 \Delta \bar{\tau} = 2, & \text{in } D, \\ \bar{\tau} = 0, & \text{on } \Gamma_k, \\ \partial \bar{\tau} \cdot n = 0, & \text{on } \Gamma_r. \end{cases} \quad (38)$$

The solution of this equation is shown in Figure 8b. We compute the expectation of  $\tau$  with DEM and CEM with the same parameters as above. The results (Figure 8a), show that the theoretical orders of convergence are not spoiled by this choice of boundary conditions. The mean order for DEM in this case is 0.55, while for CEM it is 1.15.

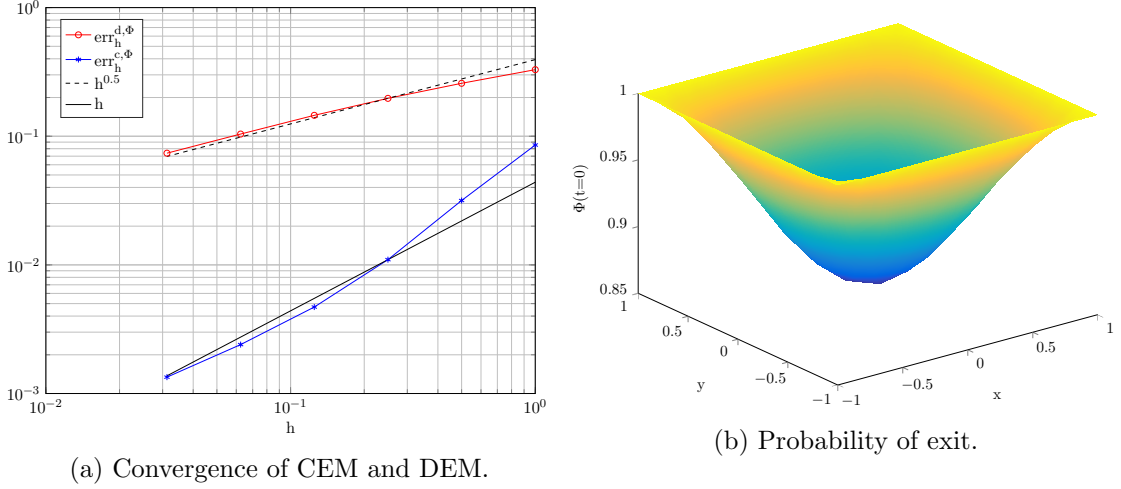


Figure 9: Summary of the results for  $\Phi$  in the two-dimensional case with pure killing boundary conditions.

#### 1.4.2 Numerical experiments - Estimation of $\Phi$

**Killing boundary conditions.** We consider the same simple case as in section 1.4.1. We consider  $\partial D$  to be a killing boundary. The solution of (1) is in this case a Brownian motion. In this case, the partial differential equation (23) reduces to

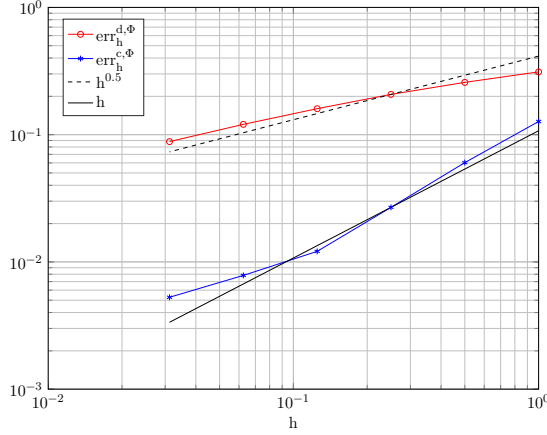
$$\begin{cases} \frac{\partial}{\partial t}\Phi(x, t, T) + \frac{1}{2}\sigma^2\Delta\Phi(x, t, T) = 0, & \text{in } D, 0 \leq t < T, \\ \Phi(x, t, T) = 1, & \text{on } \partial D, 0 \leq t < T, \\ \Phi(x, T, T) = 0, & \text{in } D. \end{cases} \quad (39)$$

We solve this problem numerically with the Finite Elements Method as for (38). The solution at  $t = 0$  is shown in Figure 9b. 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  $\Phi$  in  $(0, 0)$ , obtained by interpolation on the Finite Elements solution. The orders of convergence for this numerical experiment are shown in Figure 9a. 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.

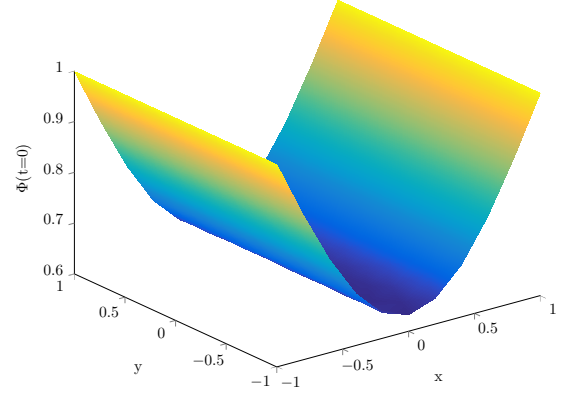
**Mixed boundary conditions.** We consider the same values for the parameters, the time integration and the Montecarlo estimation as in the pure killing case. In this case, we set the boundary conditions to be reflecting on the subset of the boundary of  $D$  defined by  $x = \pm 1$  and killing for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

$$\begin{cases} \frac{\partial}{\partial t}\Phi(x, t, T) + \frac{1}{2}\sigma^2\Delta\Phi(x, t, T) = 0, & \text{in } D, 0 \leq t < T, \\ \Phi(x, t, T) = 1, & \text{on } \Gamma_k, 0 \leq t < T, \\ \nabla\Phi(x, t, T) \cdot n = 0, & \text{on } \Gamma_r, 0 \leq t < T, \\ \Phi(x, T, T) = 0, & \text{in } D. \end{cases} \quad (40)$$

The solution of this equation computed with Finite Elements is shown in Figure 10b. The convergence results for DEM and CEM are shown in Figure 10a. The mean orders in



(a) Convergence of CEM and DEM.



(b) Probability of exit.

Figure 10: Summary of the results for  $\Phi$  in the two-dimensional case with mixed boundary conditions.

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 (40) is not negligible with respect to the error of CEM.

### 1.4.3 Numerical experiments - Adaptivity

We apply to a test case the adaptivity procedure explained in section 1.1.4. In particular, we fix  $f = 0, g = \sigma = 2, T = 10$  and  $X_0 = (0, 0)^T$  in the square domain  $[0, 1]^2$  with mixed boundary conditions. We vary the parameter  $l$  in (17) and we run DEM algorithm with  $h = h_{bound}$  for all time steps and DEM with the adaptive procedure, in order to observe the convergence of the algorithm. We expect that either choosing only the finer step size for the whole solution or using the adaptivity procedure, we will observe that the error with respect to the reference solution will be  $O(h_{int})$ . However, since in the interior zone of the domain  $D$  the step size is bigger for the adaptive method, we expect the computational cost to be smaller than for the normal DEM. Therefore, we perform a Montecarlo simulation over  $M = 10000$  trajectories, fixing  $h_0 = T$  and  $l = 4, \dots, 8$ . We estimate the mean exit time  $\bar{\tau}$  comparing it with the solution of (38). In order to measure the computational cost, we compute the average over the whole set of trajectories of the number of Euler-Maruyama steps that are performed. In Figure 11 it is possible to remark that using a wider step in the center of the domain does not spoil the order of convergence of the method while reducing the number of iterations needed to estimate the mean exit time in a non-negligible manner, especially for smaller values of the step size.

## 2 The uncertain Darcy problem

The two methods for approximating the mean exit time have been investigated in a general frame. In the following we will consider (1) with  $f: \mathbb{R}^2 \rightarrow \mathbb{R}^2$  given by the solution of the uncertain Darcy problem.

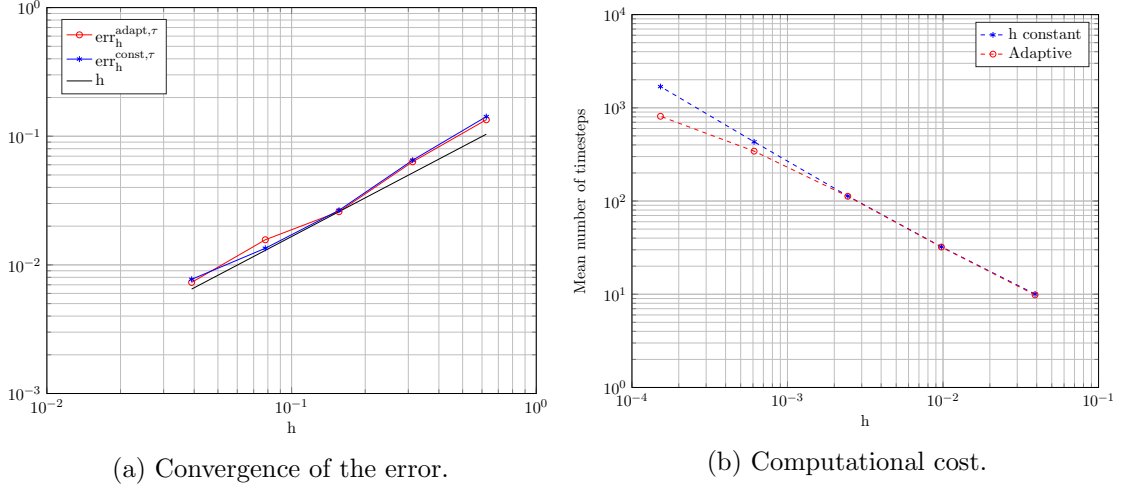


Figure 11: Estimation of  $\tau$  in the square domain with mixed boundary conditions. Comparison between DEM with fixed or adaptive step size.

## 2.1 Problem statement

Let us consider a domain  $D \subset \mathbb{R}^2$ . Let us define the Neumann boundaries of  $D$  as  $\Gamma_N$ , its inlet boundary as  $\Gamma_{in}$  and its outlet boundary as  $\Gamma_{out}$ . Then, we search the solution of the following problem

$$\left\{ \begin{array}{ll} u = -A\nabla p, & \text{in } D, \\ \nabla \cdot u = 0, & \text{in } D, \\ p = p_0, & \text{on } \Gamma_{in}, \\ p = 0, & \text{on } \Gamma_{out}, \\ \nabla p = 0, & \text{on } \Gamma_N, \end{array} \right. \quad (41)$$

where  $A$  is a random field. The solution  $u$  of this equation is used as transport field in equation (1), which can be therefore written as

$$\left\{ \begin{array}{ll} dX(t) = u(X)dt + \sigma dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D, \end{array} \right. \quad (42)$$

where we set the boundary conditions to be reflecting on  $\Gamma_N$  and killing on both  $\Gamma_{in}, \Gamma_{out}$ .

## 2.2 Finite Elements solution of the Darcy problem

Let us consider the domain  $D = [-1, 1] \times [-1, 1]$ . The random field  $A$  in (41) is chosen to be lognormal, *i.e.*,

$$A = e^\gamma, \quad (43)$$

where  $\gamma$  is a normal random field defined by its covariance function  $\text{cov}_\gamma(x_1, x_2)$  for any couple of points  $x_1, x_2$  in the domain  $D$ . The covariance function is of the Matern family, thus having the following form

$$\text{cov}_\gamma(x_1, x_2) = \frac{\sigma_A^2}{\Gamma(\nu)2^{\nu-1}} \left( \sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right), \quad \nu \geq 0.5, \quad (44)$$

where  $\sigma_A^2$  is the variance,  $L_c$  is the correlation length,  $\Gamma$  is the gamma function,  $K_\nu$  is the modified Bessel function of the second kind and  $\nu$  is a parameter. Let us remark that

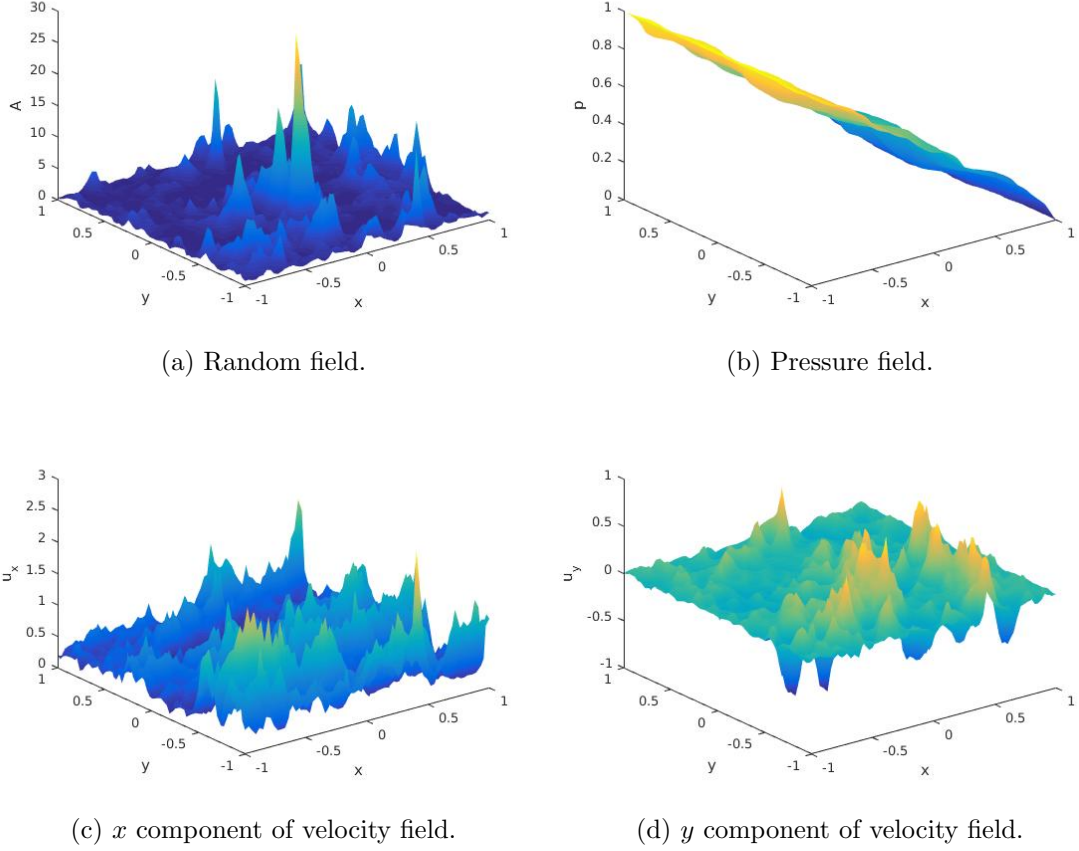


Figure 12: Approximate solution of the uncertain Darcy problem.

the covariance function does not depend on  $x_1, x_2$  but only on their euclidean distance  $|x_1 - x_2|$ . The regularity of the covariance function and of the realizations of  $A$  depend on  $\nu$ . In particular, for  $\nu$  equal to 0.5, the covariance is Lipschitz continuous and the field is  $\alpha$ -Hölder continuous for  $\alpha < 0.5$ . Results concerning further regularity properties of  $A$  can be found in [7]. The realizations of  $A$  are computed using a discrete Fourier transformation on the vertices of a grid of  $D$ , equispaced on both the  $x$  and  $y$  directions with the same spacing  $\Delta_A$ . Then, the numerical solution  $\hat{p}$  of (41) is obtained with linear Finite Elements on a regular mesh  $T_p$  with maximum element size  $\Delta_p$ . Since the vertices of the grid on which we compute  $A$  do not coincide with the vertices of  $T_p$ , we interpolate  $A$  on  $T_p$  to obtain  $\hat{p}$ . Then, the velocity field  $\hat{u}$  is retrieved computing the gradient of  $\hat{p}$ . The results for a realization of  $A$  are shown in Figure 12, where the value of the inlet pressure  $p_0$  is equal to 1, and the parameters for the random field are  $\nu = 0.5, L_c = 0.05$ .

### 2.3 Solution of the SDE

Once the Finite Element approximation  $\hat{u}$  of the velocity field is available, it is possible to approximate by means of DEM and CEM the solution of (42). The values of the numerical solution  $X_h$  can take any value in  $D$ , therefore it is necessary that the velocity field is defined in any point in  $D$ . If an interpolation of  $\hat{u}$  is performed at each step, both DEM and CEM lose in computational efficiency. Hence, an interpolation of  $\hat{u}$  has to be



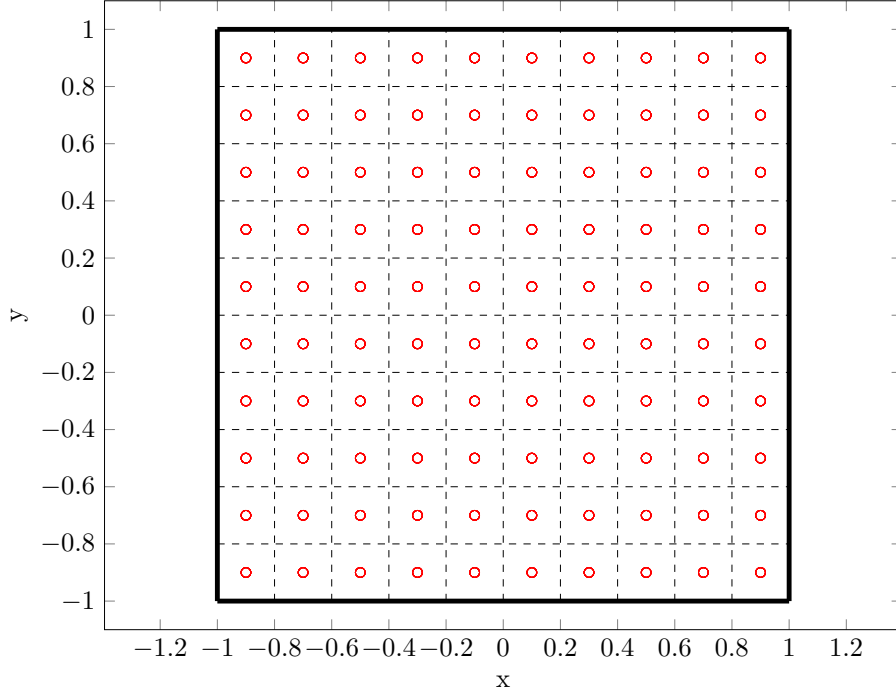


Figure 13: Grid used for interpolation of  $\hat{u}$ . The interpolation points are represented in red.

performed before the numerical integration of the SDE. Therefore, we define a grid with spacing  $\Delta_u$ , interpolating the values of  $\hat{u}$  in the center of each square defined by the grid (Figure 13). Let us denote by  $Q$  the set of the interpolation points, whose elements are defined by

$$\{Q\}_{ij} = (-1 + (i - 0.5)\Delta_u, -1 + (j - 0.5)\Delta_u)^T, \quad i, j = 1, \dots, \frac{2}{\Delta_u} =: N_u. \quad (45)$$

We compute two matrices  $U_x, U_y$  of  $\mathbb{R}^{N_u \times N_u}$  containing the values of the two components of  $\hat{u}$  interpolated on the points of  $Q$ . Then, the velocity field is considered to be piecewise constant in each square of the grid defined by  $\Delta_u$ . Therefore, if we denote by  $\tilde{u}$  the transport field for the SDE, at the  $i$ -th step of the integration  $\tilde{u}$  is evaluated as follows

$$\tilde{u}(X_h(t_i)) = \begin{pmatrix} U_x(\lceil (X_{h,1}(t_i) + 1)/\Delta_u \rceil, \lceil (X_{h,2}(t_i) + 1)/\Delta_u \rceil) \\ U_y(\lceil (X_{h,1}(t_i) + 1)/\Delta_u \rceil, \lceil (X_{h,2}(t_i) + 1)/\Delta_u \rceil) \end{pmatrix}, \quad (46)$$

where  $X_{h,1}, X_{h,2}$  denote the first and second components of  $X_h$  and  $U_x(i, j)$  represents the element  $(i, j)$  of the matrix  $U_x$  (respectively  $U_y$ ). Then, given the step size  $h$ , one step of DEM will be defined as

$$X_h(t_{i+1}) = \tilde{u}(X_h(t_i))h + \sigma(W(t_{i+1}) - W(t_i)). \quad (47)$$

Given an input initial value  $X_0$  for (42), we approximate the solution using DEM and CEM using the strategy above. In Figure 14 we display 15 trajectories for  $X_0 = (-0.8, -0.8)^T$  with two different timesteps. The choice of the initial point is made in order to observe reflections on the lower boundary of the domain  $D$  on which we compute the solution, as well as the killing boundary at the right side.

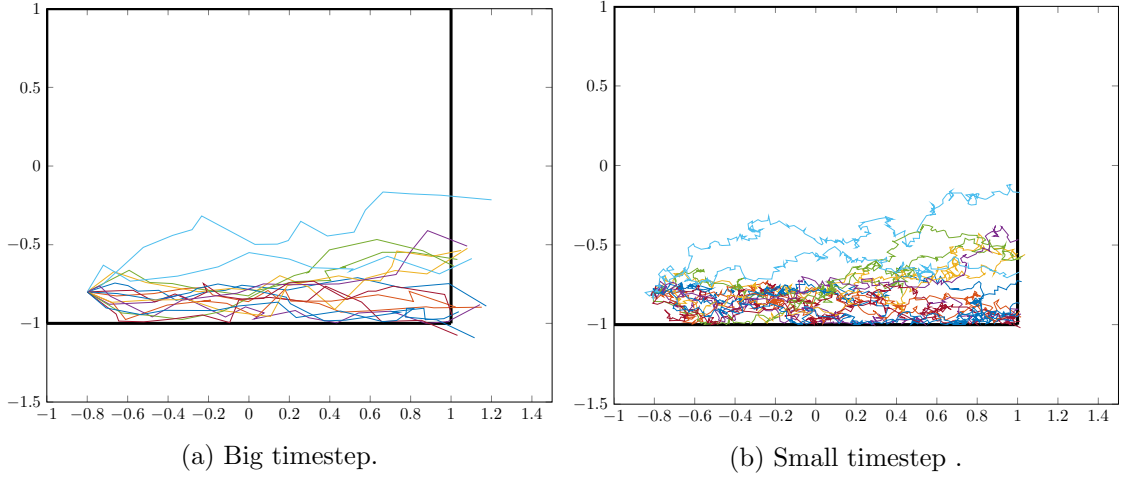


Figure 14: Trajectories of the numerical solution of (42) with DEM.

## 2.4 Summary

Let us summarize the procedure we use for approximating the solution of (42).

- Generate  $A$  on a grid with spacing  $\Delta_A$  with a Fourier transform method.
- Approximate the solution of (41) with the Finite Element methods on a fine triangulation  $T_p$  with maximum element size  $\Delta_p$ .
- Compute the velocity field from the FEM solution and interpolate it on a grid with spacing  $\Delta_u$  to obtain a piece-wise constant field  $\tilde{u}$ .
- Solve (42) with DEM or CEM to evaluate the mean exit time  $\bar{\tau}$  using  $\tilde{u}$  as the transport field.

Schematically, our procedure is the following

$$\begin{array}{ccccc}
 \text{Problem (41)} & \xrightarrow{\Delta_A} & \text{Discretized } A & \xrightarrow{\Delta_p} & \hat{p}, \hat{u} \\
 & & & & \downarrow \Delta_u \\
 & & & & \tilde{u} \\
 & & \xleftarrow[h]{} & & \\
 \bar{\tau} & \xleftarrow[\text{DEM/CEM}]{} & X_h(t_i) & & 
 \end{array}$$

## 2.5 Theoretical issues

The procedure explained above could give rise to theoretical issues concerning the existence and uniqueness of the solution of (42). In particular, when interpolating the solution  $\hat{u}$  given by FEM onto a piecewise constant function  $\tilde{u}$ , the hypothesis that the transport field of the SDE is Lipschitz continuous is not valid anymore, and therefore we have no guarantee that (42) is well-posed. On the other side, we can hope that if  $\tilde{u}$  tends uniformly to the exact solution  $u$  of (41), provided that the latter is a smooth function, the solution of the SDE that has  $\tilde{u}$  as a transport field tends to the solution given by  $u$ . In the following

we present a result in the simplified frame of a one-dimensional equation that supports our numerical procedure. Let us consider  $\sigma \in \mathbb{R}$ ,  $f: \mathbb{R} \rightarrow \mathbb{R}$  and the following SDE

$$\begin{cases} dX(t) = f(X(t))dt + \sigma dW(t), & 0 < t \leq T, \\ X(0) = X_0, \end{cases} \quad (48)$$

Moreover, let us consider a perturbation of the transport field  $f^\epsilon: \mathbb{R} \rightarrow \mathbb{R}$  and the perturbed SDE

$$\begin{cases} dX^\epsilon(t) = f^\epsilon(X^\epsilon(t)) + \sigma dW(t), & 0 < t \leq T, \\ X^\epsilon(0) = X_0. \end{cases} \quad (49)$$

We can state the following result

**Proposition 2.1.** *Given  $C, K \in \mathbb{R}$  and with the following assumptions*

1.  $|f(x) - f(y)| \leq K|x - y|, \forall x, y \in \mathbb{R}$
2.  $|f^\epsilon(x) - f(x)| \leq C, \forall x \in \mathbb{R},$
3.  $\sup_{x \in \mathbb{R}} |f(x) - f^\epsilon(x)| \xrightarrow{\epsilon \rightarrow 0} 0,$

*the solution  $X^\epsilon(t)$  of (49) converges to the solution  $X(t)$  of (48) in  $L^2(\Omega)$ , i.e.*

$$\mathbb{E}|X^\epsilon(t) - X(t)|^2 \xrightarrow{\epsilon \rightarrow 0} 0.$$

*Proof.*

$$\begin{aligned} \mathbb{E}|X^\epsilon(t) - X(t)|^2 &= \mathbb{E} \left| \int_0^t (f^\epsilon(X^\epsilon(s)) - f(X(s))) ds \right|^2 \\ &\leq T \mathbb{E} \int_0^t |f^\epsilon(X^\epsilon(s)) - f(X(s))|^2 ds \quad \{\text{Cauchy-Schwarz inequality}\} \\ &\leq T \mathbb{E} \int_0^t |f^\epsilon(X^\epsilon(s)) - f(X^\epsilon(s))|^2 ds \\ &\quad + T \mathbb{E} \int_0^t |f(X^\epsilon(s)) - f(X(s))|^2 ds \quad \{\text{Triangular inequality}\} \\ &\leq T \mathbb{E} \int_0^t |f^\epsilon(X^\epsilon(s)) - f(X^\epsilon(s))|^2 ds \\ &\quad + TK^2 \int_0^t \mathbb{E}|X^\epsilon(s) - X(s)|^2 ds. \quad \{\text{Assumption 1.}\} \end{aligned}$$

Finally, let us define

$$\alpha(t) = T \mathbb{E} \int_0^t |f^\epsilon(X^\epsilon(s)) - f(X^\epsilon(s))|^2 ds.$$

Since  $\alpha(t)$  is a non-decreasing function of  $t$ , we can apply Gronwall's inequality, which gives

$$\mathbb{E}|X^\epsilon(t) - X(t)|^2 \leq \left[ T \mathbb{E} \int_0^t |f^\epsilon(X^\epsilon(s)) - f(X^\epsilon(s))|^2 ds \right] e^{K^2 T^2}. \quad (50)$$

Assumption 2 allows us using the dominated convergence theorem, hence we can exchange the limit and the expectation. Since  $f^\epsilon$  tend uniformly to  $f$  with respect to  $\epsilon$ ,

$$\mathbb{E}|X^\epsilon(t) - X(t)|^2 \xrightarrow{\epsilon \rightarrow 0} 0.$$

□

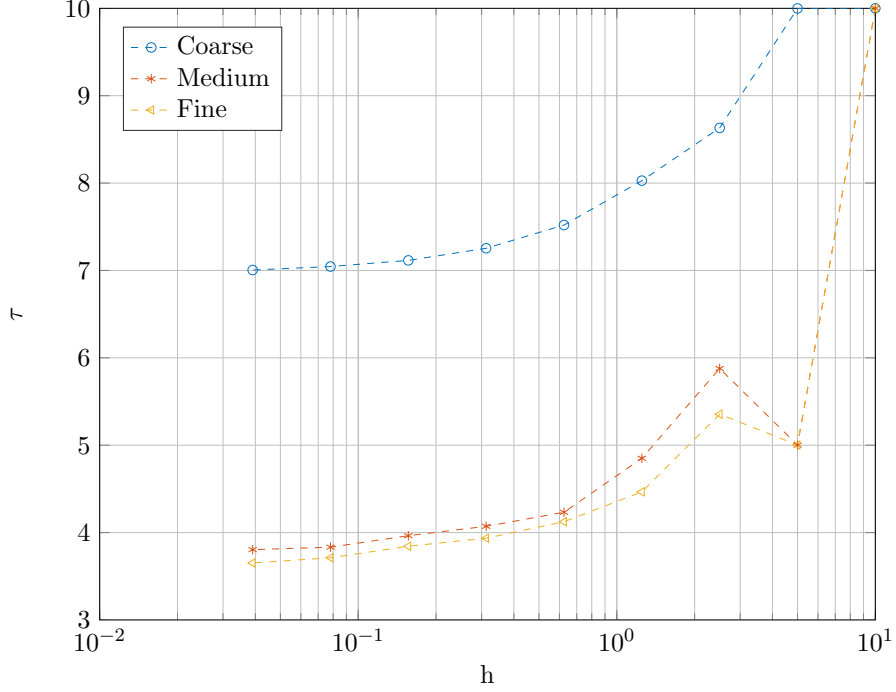


Figure 15: Results for three values of  $\Delta_A$  (coarse, medium, fine) and convergence with respect to  $h$  of the mean exit time.

Let us consider the case in which  $f^\epsilon$  is given by a piecewise constant interpolation of  $f$  on a grid with constant spacing  $\Delta_u$  over the interval  $D = [l, r] \subset \mathbb{R}$ . If  $f$  is of class  $\mathcal{C}^1$  in  $D$  the estimation (50) reduces to

$$\mathbb{E}|X^\epsilon(t) - X(t)|^2 \leq T^2 \Delta_u^2 \sup_{x \in D} |f'(x)|^2 e^{K^2 T^2} = \tilde{C} \Delta_u^2. \quad (51)$$

Hence, we could expect that the solution of the perturbed equation converges quadratically with respect to  $\Delta_u$  towards the solution of the non-perturbed SDE in the case the transport field  $f$  is sufficiently smooth.

## 2.6 Numerical Experiment - Grid refinements

We aim to verify numerically the convergence of the solution as explained in the previous section. Hence, we consider three values for  $\Delta_u$ , defining respectively a fine, medium and coarse grid, and we compute the mean exit time using CEM. We consider the parameter values  $\nu = 0.5, L_C = 0.05, \sigma_A = 1, \Delta_A = 0.0039$  for the generation of the random field  $A$ , the final time  $T = 10$ , the constant  $\sigma = 0.3$ , the step size to vary in the range  $h_i = 10/N_i, N_i = 2^i, i = 0, 1, \dots, 8$ . The values for  $\Delta_u$  are 1, 0.0625, 0.0039, for the coarse, medium and fine grids respectively. We perform a Montecarlo simulation over  $M = 50000$  trajetories in order to kill the statistical error. Results (Figure 15) show that the value of exit time converges with respect to  $h$  to approximately the same value for the medium and fine values of  $\Delta_u$ , while if the coarse interpolation is exploited, the mean exit time converges to a higher value.

## References

- [1] E. GOBET, *Weak approximation of killed diffusion using Euler schemes*, Stochastic Processes and their Applications, 87 (2000), pp. 167–197.
- [2] E. GOBET, *Euler schemes and half-space approximation for the simulation of diffusion in a domain*, ESAIM: Probability and Statistics, 5 (2001), pp. 261–297.
- [3] E. GOBET AND S. MENOZZI, *Stopped diffusion processes: boundary correction and overshoot*, Stochastic Processes and their Applications, 120 (2010), pp. 130–162.
- [4] D. S. GREBENKOV AND R. VOITURIEZ, *Exit time distribution in spherically symmetric two-dimensional domains*, (2014), pp. 1–34.
- [5] D. J. HIGHAM, X. MAO, M. ROJ, Q. SONG, AND G. YIN, *Mean Exit Times and the Multilevel Monte Carlo Method*, SIAM/ASA Journal on Uncertainty Quantification, 1 (2013), pp. 2–18.
- [6] S. KRUMSCHEID, M. PRADAS, G. A. PAVLIOTIS, AND S. KALLIADASIS, *Data-driven coarse graining in action: Modeling and prediction of complex systems*, Physical Review E, 92 (2015), p. 042139.
- [7] F. NOBILE AND F. TESEI, *A Multi Level Monte Carlo method with control variate for elliptic PDEs with log-normal coefficients*, Stochastic Partial Differential Equations: Analysis and Computations, (2015), pp. 1–47.
- [8] G. A. PAVLIOTIS, *Stochastic Processes and Applications*, 2014.
- [9] L. SIROVICH, J. E. MARSDEN, AND S. S. ANTMAN, *Theory and Applications of Stochastic Processes: An Analytical Approach*, vol. 170, Springer, 2010.