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SIMULATION**

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# **Solving Wentzell-Dirichlet Boundary Value Problem with superabundant data using reflecting random walk simulation**

**Jean-Paul MORILLON**

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**Abstract** In this paper, we are interested in numerical solution of some linear boundary value problems with Wentzell's boundary part and superabundant data on this part, by the means of simulation of reflected random walks. We use a probabilistic interpretation of solution, assuming that the diffusion coefficient and the boundary data are sufficiently smooth, and applying Itô's formula. From this stochastic representation of solution, we extend the algorithm obtained for mixed standard boundary conditions to the case of diffusion-reflection on the boundary, so called Wentzell's boundary condition. We then obtain numerical results by applying the stochastic method based upon this generalized algorithm.

**Keywords** Monte Carlo method for linear BVP · Wentzell boundary condition · Reflected diffusion · Probabilistic representation · Stochastic numerical method

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## **1 Introduction**

A large number of numerical studies have been devoted to mixed boundary value problems (BVPs) using some deterministic methods: numerical solution can be performed by the means of usual or mixed finite element methods after a variational formulation of a class of standard BVPs.

Probabilistic methods can also be relevant: see, for instance, Monte Carlo methods for Neumann and Dirichlet BVPs in [18] where the equations are discretized and specific treatments in the neighborhood of the boundary are applied.

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The aim of this paper is to investigate probabilistic numerical approach to the mixed BVP with generalized Wentzell condition on a boundary part, by the means of simulation of reflected random walks. In particular, the BVPs with Dirichlet, Neumann or Robin reflection conditions are known to have integral representations [10] which are used to obtain algorithms which compute the solution by implementing a reflected and/or absorbed random walk simulation [28,23]. In this paper, we use a probabilistic interpretation of solution, assuming that the diffusion coefficient and the boundary data are sufficiently smooth, and applying Itô's formula. From this stochastic representation of solution, we extend the algorithm obtained for mixed standard boundary conditions to the case of diffusion-reflection on the boundary, so called Wentzell's boundary condition. We then obtain numerical results by applying the stochastic method based upon this generalized algorithm.

The limitations and the main advantages of these stochastic methods are already presented, for instance, in [28,23]. In particular, the ensuing numerical methods do not require the storage of a grid discretization in computer memory, nor specific treatments related to domain local geometry. Programming is short, easy to check step by step. A contrario, the usual finite element method (FEM) leads to approximate Wentzell-Dirichlet BVP by means of a refinement of FEM on a boundary layer of thickness  $\varepsilon$  [27].

In this paper, we first introduce a Wentzell-Dirichlet BVP. Let  $G$  be a bounded open set of  $\mathbb{R}^2$  with a regular boundary  $\Gamma = \partial G$  partitioned into two boundary parts  $\Gamma_D$  and  $\Gamma_V$ :  $\Gamma = \Gamma_D \cup \Gamma_V$  and  $\Gamma_D \cap \Gamma_V = \emptyset$ .

A mixed Wentzell-Dirichlet BVP is the following one:

$$\left\{ \begin{array}{ll} -\frac{1}{2}a_G \Delta u = f & \text{in } G \\ \gamma_0 u = g_D & \text{on } \Gamma_D \\ \frac{\partial u}{\partial \nu} + \frac{1}{2}a_V \frac{\partial^2 u}{\partial \tau^2} = g_V & \text{on } \Gamma_V \end{array} \right. \quad (1)$$

where the function  $u$ , defined from  $G \subset \mathbb{R}^2$  into  $\mathbb{R}$ , is to be determined, and the data are the sufficiently smooth functions:

$$\begin{aligned} f : G &\longrightarrow \mathbb{R} & a_G : G &\longrightarrow \mathbb{R}^+ \\ g_D : \Gamma_D &\longrightarrow \mathbb{R} & a_V : \Gamma_V &\longrightarrow \mathbb{R}^+ \\ g_V : \Gamma_V &\longrightarrow \mathbb{R} \end{aligned}$$

with  $a_G > a_0 > 0$ ,  $a_V > a_0 > 0$  ( $a_0$  is a strictly positive constant), and where  $\nu$  is the inward unit normal vector and  $\tau$  is the unit tangential vector defined on  $\Gamma_V$ .

If  $\sigma_1$  is the Lebesgue measure on  $\mathbb{R}$ , then we here assume:  $\sigma_1(\Gamma_D) \neq 0$  and  $\sigma_1(\Gamma_V) \neq 0$ . When  $\Gamma$  is a polygonal boundary, we will impose the Wentzell condition at least on one straight line segment, and the Dirichlet condition on the other segments.

The boundary condition on  $\Gamma_V = \Gamma \setminus \overline{\Gamma_D}$  so called Wentzell's boundary condition [30] corresponds to the heat exchange between the body  $G$  and a thin layer of thickness  $\varepsilon$  with a thermal conductivity  $a_V/\varepsilon$ .

The body is either partially or completely covered with a highly heat-conductive thin shell, and the quantity  $u$  is then the temperature. The "heat particle" which reached the boundary at  $x \in \Gamma_V$ , diffuses on  $\Gamma_V$  just as on a boundary layer, and moves back into  $G$  along the line normal to  $\Gamma_V$  just as the rebound effect for Neumann boundary condition; then the diffusion on  $G$  takes over again [12].

This type of non-standard BVP stems from various physical phenomenae. Let us note that the same type of boundary conditions appears in absorbing boundary conditions of wave-scattering problems and, more generally, in multilayer structure problems.

Our numerical approach of Wentzell BVP is based on the limit of the following problem:

$$\left\{ \begin{array}{ll} -\frac{1}{2}a_G \Delta u = f & \text{in } G \setminus \Gamma_V^h \\ -\frac{1}{2} \frac{1}{h} a_V \Delta u = g_V^h & \text{in } \Gamma_V^h \\ \gamma u = g_D & \text{on } \Gamma_D \\ \frac{\partial u}{\partial \mathbf{v}} = g_V^v & \text{on } \Gamma_V + h/2 \\ u^+ = u^- & \text{on } \overline{G} \cap \overline{\Gamma_V^h} \\ \left( \frac{\partial u}{\partial \mathbf{v}} \right)^+ = \frac{1}{h} \left( \frac{\partial u}{\partial \mathbf{v}} \right)^- & \text{on } \overline{G} \cap \overline{\Gamma_V^h} \end{array} \right. \quad (2)$$

when  $h$  tends to 0, so that the domain  $G \cup \Gamma_V^h$  of the BVP (2) converges to the initial domain  $G$  and the BVP (2) approximates to the Wentzell-Dirichlet BVP (1), and where  $\Gamma_V^h = \{x \in \mathbb{R}^2 \mid d(x, \Gamma_V) < h/2\}$  is a boundary layer so that  $\Gamma_V^h$  is a neighborhood of  $\Gamma_V$ , and  $\Gamma_V + h/2 = \{x \in \mathbb{R}^2 \setminus (G \cup \Gamma_V^h) \mid d(x, \Gamma_V) = h/2\}$  is a boundary part of  $G \cup \Gamma_V^h$ .

The two last equalities are the transmission conditions between domain  $G$  and boundary layer  $\Gamma_V^h$ .

The extended domain  $G \cup \Gamma_V^h$  is the union of  $G$  and boundary layer  $\Gamma_V^h$ , the boundary of  $G \cup \Gamma_V^h$  is the union of  $\Gamma_D$  and  $\Gamma_V + h/2$ .

Therefore, for the functional approach of the BVP (1), we distinguish the diffusion on a boundary layer  $\Gamma_V$  and the Neumann condition on this boundary, so we consider a mixed Wentzell-Dirichlet BVP with superabundant data:

$$\left\{ \begin{array}{ll} -\frac{1}{2}a_G \Delta u = f & \text{in } G \\ \gamma u = g_D & \text{on } \Gamma_D \\ \frac{\partial u}{\partial \mathbf{v}} + \frac{1}{2}a_V \frac{\partial^2 u}{\partial \tau^2} = g_V & \text{on } \Gamma_V \\ \frac{\partial u}{\partial \mathbf{v}} = g_V^v & \text{on } \Gamma_V \end{array} \right. \quad (3)$$

where the Neumann condition on  $\Gamma_V$  is additional.

When  $\Gamma = \bigcup_{j=1}^N \overline{\Gamma_j}$  is a polygonal boundary where  $\Gamma_j$  is an open straight line segment, we consider the Wentzell condition at least on one straight line segment  $\Gamma_j$ , and we obtain the stochastic representations even if the boundary  $\partial G$  of domain  $G$  is not necessary of class  $\mathcal{C}^3$ , nor sufficiently smooth:  $\partial G$  can show corners or edges (see Section 2.).

Many situations exist in which solutions to BVP are represented as function space integrals. Such stochastic representations can be used to evaluate them numerically using Monte Carlo methods [13]. For instance, a second-order elliptic operator subject to normal reflection or to oblique derivative boundary conditions generates a diffusion process. For general definition of diffusions with reflection in a domain, see [29], and for efficient approximation, see for instance [4] and references therein. We consider here Wentzell's boundary condition corresponding to such diffusion phenomenon that a Markovian particle moves both by jumps and continuously in the state space until it dies at the time when it reaches the set where the particle is definitely absorbed.

The schedule of this paper is the following one: in Section 2, we introduce the probabilistic formulation of BVPs of Wentzell's type by means of Itô's formula associated with stochastic differential equations (SDEs). For these SDEs, we need to consider the reflecting Brownian motion and a local time on a boundary. For theoretical results on reflecting Brownian motion and on local time, see [15, 21].

Section 3 is devoted to the resolution algorithm. More precisely, the stochastic methods is introduced, and the process discretization is described. Section 4 is devoted to some numerical experiments and applications of algorithm obtained in the previous section. Finally, we present some comments in the last section.

## 2 Representation of solutions of Wentzell boundary value problem for the Laplacian

Wentzell's BVP is a model for the heat transfer between a solid  $G$  and its environment when the boundary  $\partial G$  is covered with a thin layer of a material with higher conductivity.

When  $G$  is a bounded convex domain in  $\mathbb{R}^d$ , there exists a unique solution in  $H^2(G)$  when the data are sufficiently smooth [20]. From a probabilistic point of view, when  $G$  is an open bounded set of  $\mathbb{R}^d$  with  $\mathcal{C}^3$  boundary, there exists a unique solution in  $\mathcal{C}_b^2(\overline{G})$  when the data and their derivatives are bounded and sufficiently smooth [3].

This section is devoted to the stochastic representation of solution of Wentzell's BVP by means of stochastic integrals. Let us recall that the representations according to the Robin, Neumann and mixed boundary conditions are already presented in [23, 24], and that the theoretical background can be view, for instance, in [10, 6].

Let us consider an open bounded region  $G$  in  $\mathbb{R}^d$  (the space dimension  $d$  being fixed:  $d = 2$  in this paper). Let us denote  $x \in \mathbb{R}^d$  the space variable and  $\nu$  the unit inward normal defined on the boundary  $\partial G$ .

We will show how, from stochastic differential equations, we can represent solution of Wentzell's BVP. We will use the expectation of integrals, i.e. functionals of trajectories and random variable which are solutions of SDE. The application of Itô's formula associated with SDE leads to a representation of solutions of Wentzell's BVP.

From a functional point of view, the stochastic representations of solutions of differential problems with general boundary conditions have only been obtained according to regularity hypotheses on the geometry of domain  $G$ , and on the boundary data (see [10] for the probabilistic representation of solutions of first and second BVP). In particular, the solutions are assumed of class  $\mathcal{C}_b^2(\overline{G})$ , i.e. with bounded first and second order continuous derivatives.

Nevertheless, we herein are using the stochastic representations obtained in applying Itô's formula even when the data are not necessary smooth. This procedure previously proved to be effective for the discretized equations [14,6,19], for the Dirichlet problem [28], and for the Robin, Neumann or mixed BVPs [23,24] in bi- or tridimensional domains.

More precisely, Itô's formula is used even if solutions of BVP belong to Sobolev spaces of order 1 and are not necessary of class  $\mathcal{C}_b^2(\overline{G})$ .

In the sequel, we omit the arguments  $(X_t^x(\omega))$  in the functions  $a_G, a_V, a_j$  for brevity.

## 2.1 Wentzell-Dirichlet problem

Let us consider the following bidimensional BVP:

$$\left\{ \begin{array}{ll} -\frac{1}{2}a_G \Delta u = f & \text{in } G \\ \gamma u = g_D & \text{on } \Gamma_D \\ \frac{\partial u}{\partial \mathbf{v}} + \frac{1}{2}a_V \frac{\partial^2 u}{\partial \tau^2} = g_V^v + g_V^\tau & \text{on } \Gamma_V \\ \frac{\partial u}{\partial \mathbf{v}} = g_V^v & \text{on } \Gamma_V \end{array} \right. \quad (4)$$

where the superabundant data  $g_N$  of problem (3) corresponds to  $g_V^v$  and verifies  $g_V = g_V^v + g_V^\tau$ , and where  $g_V^v$  and  $g_V^\tau : \Gamma_V \rightarrow \mathbb{R}$  are also sufficiently smooth functions.

Let us introduce the Markov process defined by the two-dimensional Laplacian operator within the domain  $G$ , by the one-dimensional Laplacian operator on the boundary part  $\Gamma_V$ , and by reflection on the boundary in the direction of inward normal  $\mathbf{v}$ .

For sake of simplicity, the initial point  $x \in G$  being fixed, we denote:  $X_t \equiv X_t^x$ ,  $\xi_t \equiv \xi_t^x$ , and  $\theta \equiv \theta^x$ , where  $X_t$  is the corresponding Markov process,  $\xi_t$  the reflection process, and  $\theta$  the hitting time of  $\mathbb{R}^d \setminus (G \cup \Gamma_V)$ .

For the bidimensional case, we have:

$$\begin{aligned} \forall t \geq 0, \\ X_t &= x + \sqrt{a_G} W_t + \int_0^t \mathbb{1}_{\Gamma_V}(X_s) \sqrt{a_V} \tau(X_s) d\beta_{\xi_s} + \int_0^t \mathbb{1}_{\Gamma_V}(X_s) \nu(X_s) d\xi_s, \\ X_0 &= x, \\ \xi_0 &= 0, \end{aligned}$$

where:

- $W_t$  is the standard Wiener process with values in  $\mathbb{R}^2$ ,
- $\beta_t$  is the standard Wiener process with values in  $\mathbb{R}$ , independent of  $W_t$ ,
- $\xi_t$  is a non decreasing process which increases only when  $t$  hits the set  $\Lambda$  defined by:  $\Lambda = \{s > 0 \mid X_s^x \in \overline{\Gamma_V}\}$ , so that:  $\xi_0 = 0$  and  $\int_0^t \mathbb{1}_G(X_s) d\xi_s = 0$ ,  $\xi_t$  is the so-called local time on  $\Gamma_V$ ,
- $\mathbb{1}_A$  is the indicator of set  $A$ ,
- $\tau$  is the unit tangential vector, and
- $\nu$  is the unit inward normal vector.

We apply Itô formula to the function  $u(X_t)$ :

$$\begin{aligned} u(X_t) - u(X_0) &= \int_0^t \mathbb{1}_G(X_s) (\nabla u(X_s), \sqrt{a_G} dW_s) + \int_0^t \frac{1}{2} a_G \Delta u(X_s) \mathbb{1}_G(X_s) ds \\ &+ \int_0^t \mathbb{1}_{\Gamma_V}(X_s) (\nabla u(X_s), \sqrt{a_V} \tau(X_s) d\beta_{\xi_s^\tau}) + \int_0^t \frac{1}{2} a_V \frac{\partial^2 u}{\partial \tau^2}(X_s) \mathbb{1}_{\Gamma_V}(X_s) d\xi_s^\tau \\ &+ \int_0^t \mathbb{1}_{\Gamma_V}(X_s) (\nabla u(X_s), \nu(X_s) d\xi_s^\nu) \end{aligned}$$

where  $\xi_s^\tau$  is the sojourn time when the process  $X_s$  diffuses on  $\Gamma_V$  and  $\xi_s^\nu$  is the local time after diffusion when the process  $X_s$  is reflected inward of  $G$ , then we use the data of problem (4):

$$\begin{aligned} u(X_t) - u(x) &= \int_0^t \mathbb{1}_G(X_s) (\nabla u(X_s), \sqrt{a_G} dW_s) - \int_0^t f(X_s) \mathbb{1}_G(X_s) ds \\ &+ \int_0^t \mathbb{1}_{\Gamma_V}(X_s) (\nabla u(X_s), \sqrt{a_V} \tau(X_s) d\beta_{\xi_s^\tau}) + \int_0^t g_V^\tau(X_s) \mathbb{1}_{\Gamma_V}(X_s) d\xi_s^\tau \\ &+ \int_0^t g_V^\nu(X_s) \mathbb{1}_{\Gamma_V}(X_s) d\xi_s^\nu \end{aligned}$$

On taking expectation of both sides of this equality, we get:

$$\begin{aligned} \mathbb{E}[u(X_t)] - u(x) &= -\mathbb{E} \left[ \int_0^t f(X_s) \mathbb{1}_G(X_s) ds \right] + \mathbb{E} \left[ \int_0^t g_V^\tau(X_s) \mathbb{1}_{\Gamma_V}(X_s) d\xi_s^\tau \right] \\ &+ \mathbb{E} \left[ \int_0^t g_V^\nu(X_s) \mathbb{1}_{\Gamma_V}(X_s) d\xi_s^\nu \right] \end{aligned}$$

The hitting time  $\theta$  of  $\mathbb{R}^d \setminus G \cup \Gamma_V$  is defined by:

$$\theta \equiv \theta^x = \inf\{t > 0 \mid X_t^x \notin G \cup \Gamma_V\}.$$

and is denoted by  $\theta$  to avoid confusion with the tangential vector  $\tau$ . We obviously assume:  $\text{Prob}\{\theta^x < \infty\} = 1$  for every  $x \in \bar{G}$  since  $a_G$  is strictly elliptic (see a similar result in [11], page 144).

The application of Itô's formula to  $u(X_t)$  leads to the following representation of the solution of (4) in the form:

$$u(x) = \mathbb{E}[R], \quad x \in G, \quad (5)$$

with the random variable:

$$\begin{aligned} R = & g_D(X_\theta) + \int_0^\theta f(X_t) \mathbb{1}_G(X_t) dt - \int_0^\theta g_V^\tau(X_t) \mathbb{1}_{\Gamma_V}(X_t) d\xi_t^\tau \\ & - \int_0^\theta g_V^v(X_t) \mathbb{1}_{\Gamma_V}(X_t) d\xi_t^v \end{aligned} \quad (6)$$

Let us mention that some functional results regarding SDE with reflection on  $\Gamma_V$ , and associated BVP with general boundary conditions are given in [8,9].

If we adopt the modified sojourn time on  $\Gamma_V$ :  $\sigma_t^\tau = \inf\{s \mid \xi_s^\tau > t\}$ , then we can write:

$$\mathbb{E} \left[ \int_0^\theta g_V^\tau(X_t) \mathbb{1}_{\Gamma_V}(X_t) d\xi_t^\tau \right] = \mathbb{E} \left[ \int_0^{\xi_\theta^\tau} g_V^\tau(X_{\sigma_t^\tau}) \mathbb{1}_{\Gamma_V}(X_{\sigma_t^\tau}) dt \right]$$

where  $X_{\sigma_t^\tau}$  is a Markov process with values in  $\Gamma_V$ ,  $t \in [0, \theta]$ ,  $\xi_t^\tau \in [\xi_0^\tau, \xi_\theta^\tau] = [0, \xi_\theta^\tau]$ , and  $\sigma_t^\tau \in [\sigma_{\xi_0^\tau}^\tau, \sigma_{\xi_\theta^\tau}^\tau] = [0, \theta]$ .

The numerical method given below in Section 3 will be based on the above expectation  $\mathbb{E} \left[ \int_0^{\xi_\theta^\tau} g_V^\tau(X_{\sigma_t^\tau}) \mathbb{1}_{\Gamma_V}(X_{\sigma_t^\tau}) dt \right]$  where the Markov process  $(X_{\sigma_t^\tau})$  diffuses on  $\Gamma_V$ , then purely and simply reflected by  $\Gamma_V$ , so the Wentzell diffusion boundary condition is considered as a degenerated elliptic equation in a boundary layer.

## 2.2 Wentzell-Dirichlet BVP in a polygonal domain

Let us denote  $G$  a bounded open set of  $\mathbb{R}^2$  with a polygonal boundary  $\Gamma = \bigcup_{k=1}^N \bar{\Gamma}_k$ , where  $\bar{\Gamma}_k$  is an open straight line segment  $]S_{k-1}, S_k[$  or  $]S_N, S_1[$ .



Let us consider the Wentzell-Dirichlet problem:

$$\left\{ \begin{array}{ll} -\frac{1}{2}a_G \Delta u = f & \text{in } G \\ \gamma_0 u = g_D & \text{on } \bigcup_{i=1}^{N_1} \overline{\Gamma_{k_i}} \\ \frac{\partial u}{\partial \mathbf{v}_j} + \frac{1}{2}a_j \frac{\partial^2 u}{\partial \tau_j^2} = g_j^{\mathbf{v}} + g_j^{\tau} & \text{on } \bigcup_{j=N_1+1}^N \Gamma_{k_j} \\ \frac{\partial u}{\partial \mathbf{v}} = g_j^{\mathbf{v}} & \text{on } \bigcup_{j=N_1+1}^N \Gamma_{k_j} \\ a_j \frac{\partial u}{\partial \tau_j} - a_{j+1} \frac{\partial u}{\partial \tau_{j+1}} = 0 & \text{on } S_j \end{array} \right. \quad (7)$$

with the superabundant data  $g_N$  of problem (3) corresponds to  $g_j^{\mathbf{v}}$ ,  $j = N_1 + 1, \dots, N$  and verifies  $g_j = g_j^{\mathbf{v}} + g_j^{\tau}$ , and where the unknown  $u$  is defined in  $G \cup \Gamma$  with real values,  $N_1$  verifies  $N_1 < N$ ,  $\mathbf{v}_j$  is the unit inward normal vector,  $\tau_j$  the unit tangential vector on  $\Gamma_{k_j}$ ,  $j = N_1 + 1, \dots, N$ , the vertices  $S_j$  exist and are defined by  $\{S_j\} = \overline{\Gamma_{k_j}} \cap \overline{\Gamma_{k_{j+1}}}$  if  $j$  and  $j+1 \in \{N_1 + 1, \dots, N\}$ , and the data  $a_G, a_j, j = N_1 + 1, \dots, N$ , are strictly positive functions so that:  $a_G \geq a_0 > 0$  and  $a_j \geq a_0 > 0, j = N_1 + 1, \dots, N$  where  $a_0$  is positive constant.

In order to avoid solutions defined up to an additive constant when the data are compatible, we assume that the interior of  $\Gamma_D$  is not empty.

The elliptic part of the boundary condition on  $\Gamma_{k_j}$  is the tangential derivative of order 2. The Wentzell boundary condition is applied on the open set  $\Gamma_V \equiv \bigcup_{j=N_1+1}^N \Gamma_{k_j}$ .

The point boundary conditions are the transmission conditions of the boundary operator.

Let us mention [20] where functional results to Wentzell BVP in a polygonal domain  $G$ . In particular, the solution  $u$  belongs to a Sobolev space of order 1.

Let us introduce the Markov process  $X_t$  with values in  $\overline{G} \subset \mathbb{R}^2$  using analogous notation:

$$\begin{aligned} \forall t \geq 0, \\ X_t &= x + \sqrt{a_G} W_t + \sum_{j=N_1+1}^N \int_0^t \mathbb{1}_{\Gamma_{k_j}}(X_s) \sqrt{a_j} \tau_j(X_s) d\beta_{\xi_s} \\ &+ \sum_{j=N_1+1}^N \int_0^t \mathbb{1}_{\Gamma_{k_j}}(X_s) \mathbf{v}_j(X_s) d\xi_s \\ &+ \sum_{j=1}^N \chi_{\mathcal{D}(\Gamma_V)} \left( \Gamma_{k_j} \cup \Gamma_{k_{j+1}} \right) \int_0^t \mathbb{1}_{S_j}(X_s) a_{\rho_j(\xi_s)}(S_j) \tau_{\rho_j(\xi_s)}(S_j) d\xi_s, \\ X_0 &= x, \\ \xi_0 &= 0, \end{aligned}$$

where  $\chi_{\mathcal{P}(\Gamma_V)}(B)$  equals to 1 if  $B$  is a part of  $\Gamma_V$ , 0 otherwise, and  $\rho_k$  is the uniform distribution on  $\{k, k+1\}$  so that:  $\text{Prob}\{\rho_k(\xi_s) = k\} = \text{Prob}\{\rho_k(\xi_s) = k+1\} = \frac{1}{2}$ ,  $k = 1, \dots, N-1$ , and  $\text{Prob}\{\rho_N(\xi_s) = N\} = \text{Prob}\{\rho_N(\xi_s) = 1\} = \frac{1}{2}$ .

As above, this process  $X_t$  is absorbed by  $\Gamma_D$  at the hitting time  $\theta$  defined by:

$$\theta = \inf\{t > 0 \mid X_t \in \Gamma_D\}.$$

The application of Itô's formula to  $u(X_t)$  leads to the following representation of the solution of (7) in the form:

$$u(x) = \mathbb{E}[R], \quad x \in G, \quad (8)$$

with the random variable:

$$R = g_D(X_\theta) + \int_0^\theta f(X_t) \mathbb{1}_G(X_t) dt - \sum_{j=N_1+1}^N \int_0^\theta g_j^\tau(X_t) \mathbb{1}_{\Gamma_{k_j}}(X_t) d\xi_t^\tau - \sum_{j=N_1+1}^N \int_0^\theta g_j^v(X_t) \mathbb{1}_{\Gamma_{k_j}}(X_t) d\xi_t^v \quad (9)$$

The problem (7) can be written in the following condensed form, using appropriate values of coefficients  $\alpha$ ,  $\beta$ , and  $\gamma$ :

$$\left\{ \begin{array}{ll} -\frac{1}{2} a_G \Delta u = f & \text{in } G \\ \beta \frac{\partial u}{\partial \nu} + \frac{1}{2} \alpha \frac{\partial^2 u}{\partial \tau^2} - \gamma u = g & \text{on } \Gamma = \partial G \end{array} \right. \quad (10)$$

Let us note the analogy between problems (7) and (10). Nevertheless, from the functional point of view, some difficulties occur since the coefficients  $\alpha$ ,  $\beta$  and  $\gamma$  are discontinuous. Some partial results on this subject can be found in [3, 26].

In the next section of this paper, we will focus on one stochastic method based upon the probabilistic representation of solution of BVP (7).

### 3 Resolution algorithm for Wentzell-Dirichlet mixed boundary value problem

The main purpose of this section is to give an approach of the representations of Section 2 by means of realization of random processes, in order to compute the solutions of BVP with a Wentzell boundary part.

Let us recall that some efficient algorithms according to the Dirichlet, Neumann, Robin and mixed boundary conditions are already presented in [28, 23] for the Laplacian and in [24] for the parabolic operator. Our present aim is then to extend the above techniques to our problem (7).

In order to estimate an expectation  $\mathbb{E}[R]$ , we simulate a large number (say  $NT$ ) of independent random variables with the same law as  $R$ . The mean of the  $NT$  realizations  $R_i$  converges almost surely to  $\mathbb{E}[R]$  (see [13] where the almost sure convergence of the Monte Carlo methods is proved):

$$\frac{1}{NT} \sum_{i=1}^{NT} R_i \xrightarrow{a.s.} \mathbb{E}[R] \quad \text{as } NT \rightarrow +\infty.$$

Thanks to CLT, the rate of convergence of this approximation is known, it is of order  $1/\sqrt{NT}$ .

In order to simulate the diffusion process  $X$ , we approach  $X$  by means of an Euler's scheme as in [1, 2, 24] or the Box Muller algorithm. We need also the simulation of random walks by using some predefined generators of normally distributed pseudorandom numbers.

Let us consider the Wentzell-Dirichlet BVP (7) in a polygonal domain.

The solution  $u(x)$  to BVP (7) is represented as the mean of a random variable  $R$ , involving function of a non instantaneously reflected random walk, then absorbed random walk.

The representation (8)–(9) is used and  $u(x)$  is computed as the mean of  $NT$  approximated values of  $R$ , i.e.  $R_1, \dots, R_{NT}$ , in order to obtain an estimation of  $u(x)$ :

$$u(x) \simeq \frac{1}{NT} \sum_{i=1}^{NT} R_i.$$

Each value  $R_i$  results from a simulation of a random walk on  $G$ , first reflected by the Wentzell boundary part  $\Gamma_V$ , then absorbed by the Dirichlet boundary part  $\Gamma_D$ . Each random walk is then finite. From now on, we shall assume that the hitting time  $\theta$  is not too large and, in particular, the Dirichlet boundary part  $\Gamma_D$  versus the Wentzell boundary part  $\Gamma_V$  is significant.

The standard Wiener processes are simulated as follows. The mean of space step  $h > 0$  being fixed, the process  $W_t$  can be simulated by the sequence of random vectors  $W_0, W_1, \dots, W_j$  defined by means of the recurrent formulae:

$$W_0 = x \in G, \quad \text{and} \quad W_{j+1} = W_j + hD_j, \quad j \in \mathbb{N},$$

where  $D_j$  is a random vector so that, if  $(e_i, i = 1, 2)$  is the canonical basis of  $\mathbb{R}^2$ ,  $D_j$  verifies:

$$D_j = r_1 e_1 + r_2 e_2 \quad \text{in } G$$

where  $r_1$  and  $r_2$  are independent normally distributed pseudorandom numbers, and:

$$D_j = r_3 \tau + |r_4| \nu \quad \text{on } \Gamma_V$$

where  $r_3$  and  $r_4$  are independent normally distributed pseudorandom numbers.

The absolute value  $|r_4|$  leads to a reflection inward  $G$ .

Since the simulated process happens to leave the domain  $G$ , its trajectory resumes to the interior after a diffusion on  $\Gamma_V$  or stops when the trajectory hits the Dirichlet boundary part  $\Gamma_D$ .

The process is not instantaneously reflected by the boundary part  $\Gamma_V$  when diffusion occurs. The elementary boundary reflections without diffusion are detailed in [24], where the basic reflection algorithm is given, and general obliquely reflected diffusions (without diffusion on the boundary) are studied in [4]. The diffusion on the Wentzell boundary part is governed by the Wiener process  $\beta_t$  which is simulated as the process  $W_t$  but on the boundary layer:

$$\Gamma_V^h = \{x \in \mathbb{R}^2 \mid d(x, \Gamma_V) < h/2\}.$$

In the bidimensional case, the process diffuses on  $\Gamma_V$ , along the tangential line given by  $\tau$ , and is reflected inward the interior  $G$  along the normal direction given by  $\nu$ .

Each simulation gives a discrete realization  $(X_j, 0 \leq j \leq NP)$  of a random walk in  $G$  with  $NP$  steps, so that:

$$X_0 \in \overline{G} \setminus \Gamma_D, \dots, X_{NP-1} \in \overline{G} \setminus \Gamma_D, \quad \text{and} \quad X_{NP} \in \Gamma_D^h = \{x \in \mathbb{R}^2 \mid d(x, \Gamma_D) < h/2\},$$

which trajectory is the polygonal line connecting successively the points  $X_j$  and  $X_{j+1}$ ,  $j = 0, \dots, NP - 1$ , in order to form a random path.

The random processes are discretized in time according to the Euler scheme.

For each simulated random walk  $(X_j, 0 \leq j \leq NP)$ , we compute the score:

$$\begin{aligned} R_i = & g_D(X_{NP}) + \Delta t \cdot \sum_{j=0}^{NP-1} f(X_j) - \Delta s \cdot \sum_{j=0}^{NP-1} g_V^\tau(X_j) \mathbb{1}_{\Gamma_V^h}(X_j) \\ & - \Delta W \cdot \sum_{j=0}^{NP-1} g_V^\nu(X_j) \mathbb{1}_{\Gamma_V^h}(X_j) \end{aligned}$$

where  $\Delta t$  is the time of a step in  $G$ ,  $\Delta s$  is the local time of a step along  $\tau$  on  $\Gamma_V^h$ , and  $\Delta W$  is the step increment along  $\nu$ .

Then this procedure is iterated  $NT$  times in order to obtain a sample of  $R$ , and an estimation of its arithmetic mean  $u(x)$ .

The integer  $NT$  corresponds to the number of simulated random walks, and consequently to the number of absorptions by the Dirichlet boundary part  $\Gamma_D$ , more precisely by  $\Gamma_D^h$ .

This integer  $NT$  is the maximum index of the main loop of the associated program. The second (and latter) loop follows, step by step, each random walk by adding up successively the values of the source function  $f$ , and the values of the Wentzell condition  $g_V$  by diffusion and the values of the Neumann condition by straight reflection, then the value of the absorption effect  $g_D$ . Finally the score of each corresponding  $R_i$  is added up.

For each realization of the random variable  $R$ , we generate:

1. a first random walk in the open set  $G$ , depending on the Wiener process  $W_t$  (see, for instance, the simplest random walk in [28]),
2. a second random walk on the boundary part  $\Gamma_V$ , depending on the Wiener process  $\beta_t$  which is simulated as the process  $W_t$  extended on the boundary layer  $\Gamma_V^h$ , and
3. a reflection by  $\Gamma_V$  along the inward normal  $\nu$ .

If  $h$  is the fixed average of stepsize of a simulated bidimensional walk  $X_j$ , the time and space increments are defined by:

$$\Delta t = \frac{h^2}{a_G} \text{ in } G, \quad \Delta s = \frac{h^2}{2a_V} \text{ on } \Gamma_V^h, \quad \Delta W = h \text{ inward along } \nu.$$

If  $a_V \equiv 0$ , then the random walk is instantaneously reflected by the boundary  $\Gamma_V$  as in [23] for the Neumann BVP. Else  $a_V \neq 0$ , we have a diffusion on  $\Gamma_V$  and a mirror effect: the random walk diffuses on  $\Gamma_V$  and resumes to the interior; this procedure goes on until the trajectory reaches the Dirichlet boundary part  $\Gamma_D$ .

*Remark 1* When  $X_t$  hits the boundary part  $\Gamma_V$  by means of the Wiener process  $W_t$ , then  $(W \cdot \tau)\tau$  is replaced by  $\beta\tau$  and  $(W \cdot \nu)\nu$  by  $|W \cdot \nu|\nu$ , i.e. if  $X_t \in \Gamma_V$ , then

$$X_{t+dt} = X_t + \sqrt{a_V} \tau(X_t) d\beta_{\xi_t} + \sqrt{a_V} |dW_t \cdot \nu| \nu$$

where  $\cdot$  is the scalar product in the euclidean space  $\mathbb{R}^2$  and:

$$|dW_t \cdot \nu| = \text{sgn} [(X_t + dW_t) \cdot \nu] (dW_t \cdot \nu)$$

(see [10], page 85 for the relation between the positive process  $|x + W_t|$  in  $\mathbb{R}^+$  and the local time  $\xi_t$  at zero).

*Remark 2* In our algorithm (see the pseudo-code shown below, page 13), we can use antithetic random variables with the same distribution to estimate  $u$  and improve its variance.

Two processes  $W_t^{(1)}$  and  $W_t^{(2)}$  are simulated by the two sequences of random vectors  $W_0, W_1^{(1)}, \dots, W_j^{(1)}$  and  $W_0, W_1^{(2)}, \dots, W_j^{(2)}$  defined by means of the recurrent formulae:

$$W_0 = x \in G, \quad W_{j+1}^{(1)} = W_j^{(1)} + hD_j^{(1)}, \quad \text{and} \quad W_{j+1}^{(2)} = W_j^{(2)} + hD_j^{(2)} \quad j \in \mathbb{N},$$

where  $D_j^{(1)}$  and  $D_j^{(2)}$  are random vectors so that, if  $(e_i, i = 1, 2)$  is the canonical basis of  $\mathbb{R}^2$ ,  $D_j^{(1)}$  and  $D_j^{(2)}$  verify:

$$D_j^{(1)} = r_1 e_1 + r_2 e_2 \quad \text{and} \quad D_j^{(2)} = -D_j^{(1)} \quad \text{in } G$$

where  $r_1$  and  $r_2$  are independent normally distributed pseudorandom numbers, and:

$$D_j^{(1)} = r_3 \tau + |r_4| \nu \quad \text{and} \quad D_j^{(2)} = -r_3 \tau + |r_4| \nu \quad \text{on } \Gamma_V$$

where  $r_3$  and  $r_4$  are independent normally distributed pseudorandom numbers, independent of  $r_1$  and  $r_2$ .

When a process  $W_t^{(i)}$  is absorbed by  $\Gamma_D$ , the second  $W_t^{(j)}$ ,  $j \neq i$ , continues until it also reaches  $\Gamma_D$ .

For each simulated random walk  $(X_j; 0 \leq j \leq NP)$ , we compute the score:

$$\begin{aligned} R_i = & g_D(X_{NP}) + \frac{h^2}{a_G} \sum_{j=0}^{NP-1} f(X_j) \mathbb{1}_G(X_j) - \frac{h^2}{2a_V} \sum_{j=0}^{NP-1} g_V^\tau(X_j) \mathbb{1}_{\Gamma_V^h}(X_j) \\ & - h \sum_{j=0}^{NP-1} g_V^\nu(X_j) \mathbb{1}_{\Gamma_V^h}(X_j) \end{aligned}$$

We then estimate  $u(x)$  by computing the arithmetic mean of these  $NT$  scores  $R_i$ .

A pseudo-code description of the global algorithm can be written as follows:

Declarations — Initializations, diffusion coefficient  $a_V$  on Wentzell boundary part  $\Gamma_V$  included

Loop Points of domain  $G$  grid

Set initial point  $x$  of the domain grid

Main Loop  $i = 1, \dots, NT$  random walks from  $x$  to Dirichlet boundary part  $\Gamma_D$

Let  $j = NT + i$  for the antithetic random walks

Initialize for each random walk:

Start points of antithetic random walks:  $W_i = x; W_j = x$

Source function  $f$  effect in domain  $G$ :  $ya_i = 0.0$  and  $ya_j = 0.0$

Wentzell diffusion effect on  $\Gamma_V$ :  $maV_i = 0.0$  and  $maV_j = 0.0$

Neumann effect on  $\Gamma_V$ :  $maN_i = 0.0$  and  $maN_j = 0.0$

While the random walks  $W_i$  and  $W_j$  within the domain  $G$  (Loop step by step)

Source function  $f$  effect at points  $W_i$  and  $W_j$ :

$ya_i = ya_i + f(W_i)$  and  $ya_j = ya_j + f(W_j)$

Set  $D_i$  a normally distributed pseudo-random vector

Set  $r$  a normally distributed pseudo-random number

If  $W_i$  on Wentzell boundary  $\Gamma_V$

$W_i = W_i + hr\tau$

Diffusion effect:  $maV_i = maV_i + g_V(W_i)$

Reflection of random walk inside  $G$  with Neumann effect:

$maN_i = maN_i + g_N(W_i)$

endIf

If  $W_j$  on Wentzell boundary  $\Gamma_V$

$W_j = W_j - hr\tau$

Diffusion effect:  $maV_j = maV_j + g_V(W_j)$

Reflection of random walk inside  $G$  with Neumann effect:

$maN_j = maN_j + g_N(W_j)$

endIf

$W_i = W_i + hD_i$ , i.e. a step of first random walk

$W_j = W_j - hD_i$ , i.e. a step of second random walk

endWhile the random walks  $W_i$  and  $W_j$  within the domain  $G$  (Loop step by step)

Comment: Dirichlet condition: absorption of  $W_i$  or  $W_j$  by  $\Gamma_D$

If  $W_i \in \Gamma_D$

$maU(x, i) = g_D(W_i) - 0.5h^2/a_V maV_i - hmaN_i$

endIf

If  $W_j \in \Gamma_D$

$maU(x, j) = g_D(W_j) - 0.5h^2/a_V maV_j - hmaN_j$

endIf

Comment: Continue with the unabsorbed walk  $W_i$  or  $W_j$

If  $W_j \in \Gamma_D$

While  $W_i \notin \Gamma_D$

$ya_i = ya_i + f(W_i)$

Set  $D_i$  and  $r$  normally distributed pseudo-random vector and number

If  $W_i$  on Wentzell boundary  $\Gamma_V$

```

         $W_i = W_i + hr\tau$ 
        Diffusion effect:  $maV_i = maV_i + g_V(W_i)$ 
        Reflection of random walk inside  $G$  with Neumann effect:
         $maN_i = maN_i + g_N(W_i)$  ;
    endif
     $W_i = W_i + hD_i$  A step of first random walk
endWhile  $W_i \notin \Gamma_D$ 
If  $W_i \in \Gamma_D$ 
     $maU(x, i) = g_D(W_i) - 0.5h^2/a_V maV_i - hmaN_i$ 
endif
endIf  $W_j \in \Gamma_D$ 
If  $W_i \in \Gamma_D$ 
    While  $W_j \notin \Gamma_D$ 
         $ya_j = ya_j + f(W_j)$ 
        Set  $D_j$  and  $r$  normally distributed pseudo-random vector and number
        If  $W_j$  on Wentzell boundary  $\Gamma_V$ 
             $W_j = W_j + hr\tau$ 
            Diffusion effect:  $maV_j = maV_j + g_V(W_j)$ 
            Reflection of random walk inside  $G$  with Neumann effect:
             $maN_j = maN_j + g_N(W_j)$  ;
        endif
         $W_j = W_j + hD_j$  A step of second random walk
    endwhile  $W_j \notin \Gamma_D$ 
    If  $W_j \in \Gamma_D$ 
         $maU(x, j) = g_D(W_j) - 0.5h^2/a_V maV_j - hmaN_j$ 
    endif
endIf  $W_i \in \Gamma_D$ 
Add source effect and boundary conditions:
1)  $maU(x, i) = maU(x, i) + h^2/a_G ya_i$  for the first random walk  $W_i$ 
2)  $maU(x, j) = maU(x, j) + h^2/a_G ya_j$  for the antithetic random walk  $W_j$ 
end Main Loop  $i = 1, \dots, NT$  random walks from  $x$  to Dirichlet boundary part  $\Gamma_D$ 
Calculate estimated solution (arithmetic mean):  $u(x) = \frac{1}{2NT} \sum_{k=1}^{2NT} maU(x, k)$ 
 $U(x) = \text{mean}\{maU(x, k) \mid 1 \leq k \leq 2NT\}$ 
Display per point approximated solution, empirical errors, standard deviation and
95% confidence intervals
endLoop Points of domain  $G$  grid

```

#### 4 Numerical experiments

The validity and suitability of the present approach, i.e. the stochastic representation in Section 2 and the approximate solution in Section 3, are investigated here by considering and evaluating a set of BVPs with Wentzell's boundary condition according to the above numerical scheme used sequential calculus on personal computers (Intel i7 CPU 2.67 GHz, and Athlon 2850e 1.80 GHz) by the means of MATLAB® applications.

In all the following examples, the solution  $u$  is approximated by  $u_c$  in  $NPT$  points  $Q_1, Q_2, \dots, Q_{NPT}$  in  $\bar{G}$ .

The quality of the stochastic approximation is controlled as follows:

$$\begin{aligned} ER_{\max} &= \max \{ ER_i : 1 \leq i \leq NPT \} \\ ER_i &= \frac{10 |u(Q_i) - u_c(Q_i)|}{1 + 10 |u(Q_i)|} \end{aligned}$$

so that  $ER_i, i = 1, \dots, NPT$ , furnish relative errors or absolute errors, according to the magnitude of the theoretical value.

The following examples show BVP (7), one defined in a rectangular domain  $G = ]0, a[ \times ]0, b[$ , and two in the unit square  $G = ]0, 1[^2$ . The fourth example shows BVP (4) defined in quadrant of ring  $G = D(0; 3) \setminus D(0; 1) \cap (\mathbb{R}^{*+} \times \mathbb{R}^{*+})$ . For sake of simplicity, the diffusion coefficient  $a_G$  in  $G$  equals to 1.

#### 4.1 Wentzell-Dirichlet mixed BVP in a rectangular domain

Let us consider problem (7) in  $G = ]0, a[ \times ]0, b[$  with the following data:

$$\begin{aligned} f &\equiv 0 && \text{in } G \\ \Gamma_D &= ([0, a] \times \{0\}) \cup ([0, a] \times \{b\}) \\ g_D(x, 0) &= 0 && \text{on } [0, a] \times \{0\} \\ g_D(x, b) &= \cos^2(\pi x/a) && \text{on } [0, a] \times \{b\} \\ \Gamma_V &= (\{0\} \times ]0, b[) \cup (\{a\} \times ]0, b[) \\ g_V^x(x, y) &= a_V \frac{\pi^2 \sinh(2\pi y/a)}{a^2 \sinh(2\pi b/a)} && \text{on } \Gamma_V \\ g_V^y(x, y) &= 0 && \text{on } \Gamma_V \end{aligned}$$

such that this Wentzell-Dirichlet BVP admits a unique solution  $u$  written in the form:

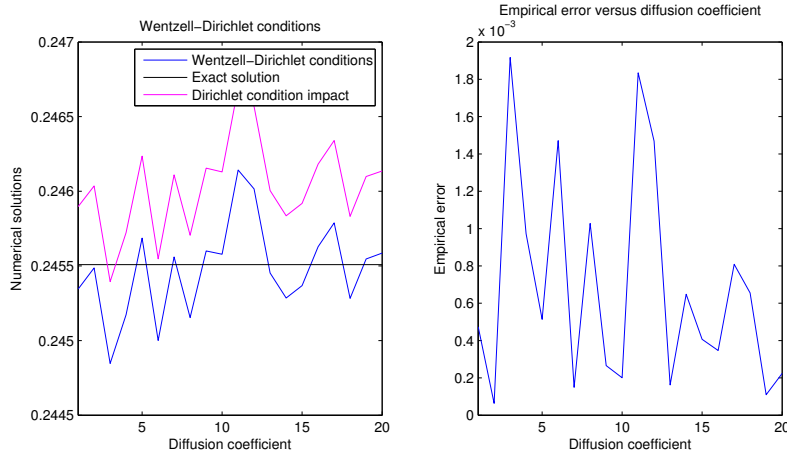
$$u(x, y) = \frac{y}{2b} + \cos(2\pi x/a) \frac{\sinh(2\pi y/a)}{2 \sinh(2\pi b/a)}.$$

Let us first consider the point  $(a/2, b/2)$  and the solution  $u(a/2, b/2)$  for different values of diffusion coefficient  $a_V$  on  $\Gamma_V$ :  $a_V \in \{1, \dots, 20\}$ .

The results of the mean value of the approximate solution  $u(a/2, b/2)$  are obtained with the following data:

1. Rectangular domain:  $a = 2$  and  $b = 3$
2. Number of random walks:  $NT = 6 \times 10^4$ , i.e.  $2NT = 12 \times 10^4$  by means of anti-thetic variables
3. Stepsize of each random walk:  $h = 0.01$





**Fig. 1** Numerical solution  $u(a/2, b/2)$  and empirical error versus  $a_V$

The arithmetic mean of these  $2NT$  scores  $R_i$  gives:  $u(a/2, b/2) \simeq 0.2455$ , the standard deviation  $\sigma = 0.1775$  is obtained by means of antithetic variables, and 95% confidence intervals  $[u_c - 1.96\sigma/\sqrt{2NT}, u_c + 1.96\sigma/\sqrt{2NT}]$ , around  $u_c = 0.2455$ , is of amplitude 0.028.

The empirical error for the Wentzell diffusion coefficient  $a_V$  :

$$ER_{a_V}(a/2, b/2) = \frac{10 |u(a/2, b/2) - u_c(a/2, b/2)|}{1 + 10 |u(a/2, b/2)|}$$

is less than  $2 \times 10^{-3}$  and verifies:

$$\max_{1 \leq a_V \leq 20} ER_{a_V}(a/2, b/2) \simeq 1.9 \times 10^{-3} \quad \text{and} \quad \frac{1}{20} \sum_{a_V=1}^{20} ER_{a_V}(a/2, b/2) \simeq 0.8 \times 10^{-3}.$$

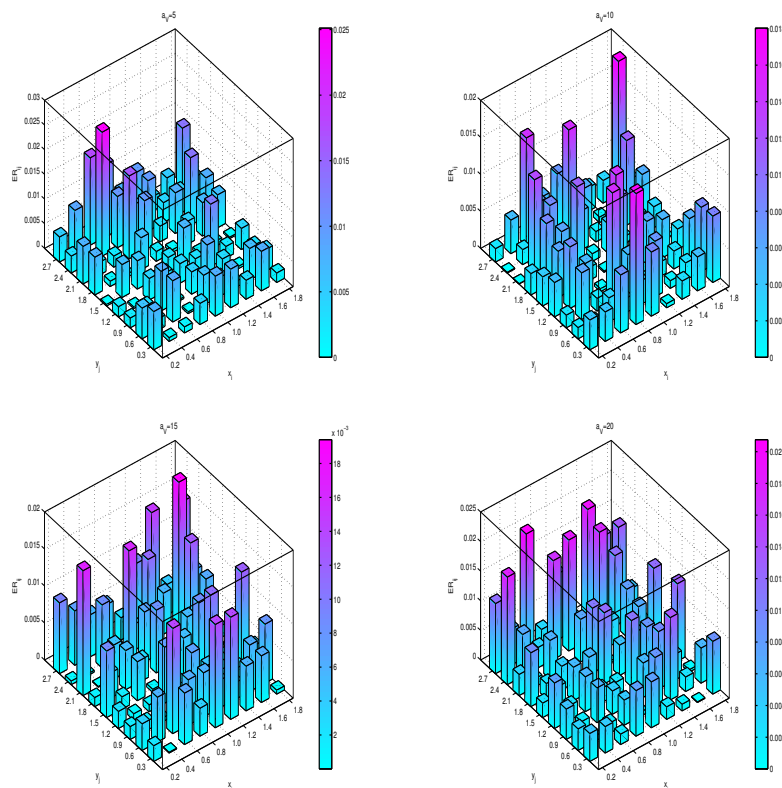
See figure 1 where numerical solutions and empirical errors are represented versus  $a_V$ . The effect of Dirichlet condition is isolated, so we can appreciate the effect of diffusion on  $\Gamma_V$ .

Let us secondly consider the points  $Q_{ij} = Q(x_i, y_j)$ , where  $x_i = 0.1 \times a \times i$ ,  $1 \leq i \leq 9$ ,  $y_j = 0.1 \times b \times j$ ,  $1 \leq j \leq 9$ , the approximated solution  $u_c(Q_{ij})$ , the empirical errors  $ER_{ij}$  at the point  $Q(x_i, y_j)$ , and  $ER_{\max}$  when the boundary diffusion coefficient  $a_V$  belongs to  $\{5, 10, 15, 20\}$ .

The values of  $ER_{\max}$  given in Table 1 are obtained with the number of simulated random walks:  $NT = 2 \times 10^5$  and the data above, and the empirical errors  $ER_{ij}$  are given in Figure 2.

**Table 1** Maximum empirical errors for different  $a_V$ 

$a_V$	$ER_{\max}$	at point $(x_i, y_i)$
5	0.0251	at (0.6;2.4)
10	0.0180	at (1.8;2.7)
15	0.0194	at (1.6;2.4)
20	0.0208	at (0.6;2.7)

**Fig. 2** Empirical errors in rectangular domain for  $a_V = 5, 10, 15, 20$ 

#### 4.2 Wentzell-Dirichlet mixed BVPs in the unit square

Let us consider two problems (7) in  $G = ]0, 1[{}^2$  where the Dirichlet and Wentzell boundary parts  $\Gamma_D$  and  $\Gamma_V$  are:

$$\Gamma_D = ([0, 1] \times \{0\}) \cup ([0, 1] \times \{1\}) \quad \text{and} \quad \Gamma_V = (\{0\} \times ]0, 1]) \cup (\{1\} \times ]0, 1]),$$

and with the following data:

First problem  $P_1$  in the unit square:

$$\begin{aligned} f &\equiv -2 && \text{in } G \\ g_D(x, 0) &= x^2 + 1 && \forall x \in [0, 1] \\ g_D(x, 1) &= x^2 && \forall x \in [0, 1] \\ g_V^\tau &\equiv a_V && \text{on } \Gamma_V \\ g_V^v(0, y) &= 0 && \forall y \in ]0, 1[ \\ g_V^v(1, y) &= -2 && \forall y \in ]0, 1[ \end{aligned}$$

such that this first Wentzell-Dirichlet BVP  $P_1$  admits a unique solution  $u$  written in the form:

$$u(x, y) = x^2 + (y - 1)^2.$$

Second problem  $P_2$  in the unit square:

$$\begin{aligned} f &\equiv 0 && \text{in } G \\ g_D(x, 0) &= \cos(\pi x) && \forall x \in [0, 1] \\ g_D(x, 1) &= \cos(\pi x) \exp(\pi) && \forall x \in [0, 1] \\ g_V^\tau(0, y) &= \frac{1}{2} a_V \pi^2 \exp(\pi y) && \forall y \in ]0, 1[ \\ g_V^\tau(1, y) &= -\frac{1}{2} a_V \pi^2 \exp(\pi y) && \forall y \in ]0, 1[ \\ g_V^v &\equiv 0 && \text{on } \Gamma_V \end{aligned}$$

such that this second Wentzell-Dirichlet BVP  $P_2$  admits a unique solution  $u$ :

$$u(x, y) = \cos(\pi x) \exp(\pi y).$$

Let us consider the points  $Q_{ij} = Q(x_i, y_j)$ , where  $x_i = 0.1 \times i$ ,  $1 \leq i \leq 9$ ,  $y_j = 0.1 \times j$ ,  $1 \leq j \leq 9$ , the approximated solution  $u_c(Q_{ij})$ , the empirical errors  $ER_{ij}$  at the point  $Q(x_i, y_j)$ , and  $ER_{\max}$  when the boundary diffusion coefficient  $a_V$  belongs to  $\{5, 10, 15, 20\}$ .

The value of  $ER_{\max}$  and the mean of ER given in Table 2 for problem  $P_1$  and in Table 3 for problem  $P_2$  are obtained with the following data:

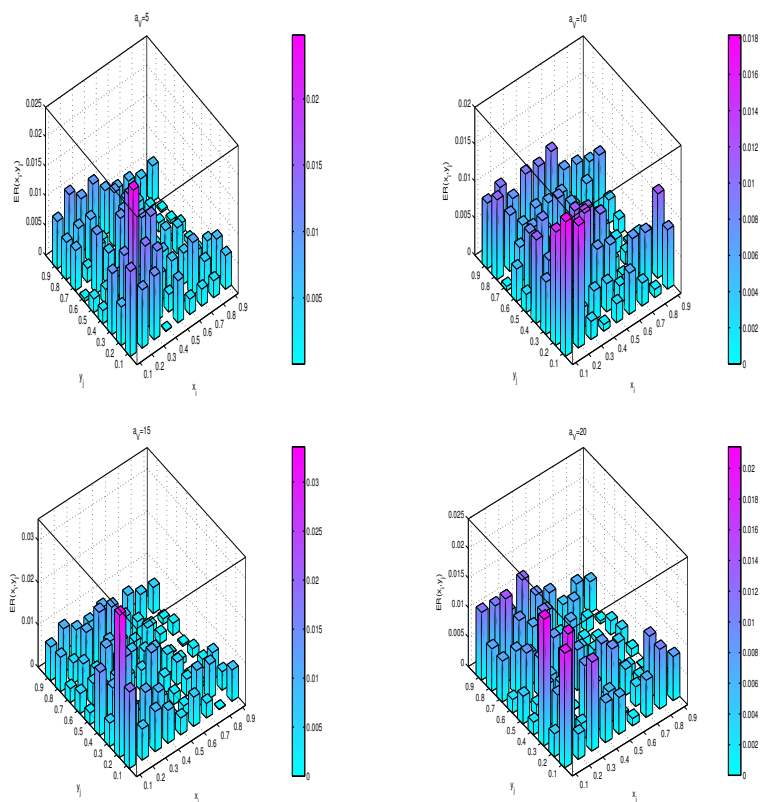
1. Number of simulated random walks:  $NT = 6 \times 10^4$ , i.e.  $2NT = 12 \times 10^4$  by means of antithetic variables
2. Stepsize of each random walk:  $h = 0.01$

and the empirical errors  $ER_{ij}$  are given in Figure 3 for problem  $P_1$  and in Figure 4 for problem  $P_2$ .

For the BVP  $P_2$ , the maximum error  $ER_{\max}$  is obviously where the exact solution equals to zero (the results in Figure 4 where the zero points are clearly identified, confirm this effect due to the choice of the expression of  $ER_{\max}$ ); for these points, the maximum error is equal to 10 times the absolute error and the 95% confidence intervals given in Table 4 always contain the exact solution  $u = 0$ .

**Table 2** BVP  $P_1$ : Maximum empirical error and error mean for different  $a_V$ 

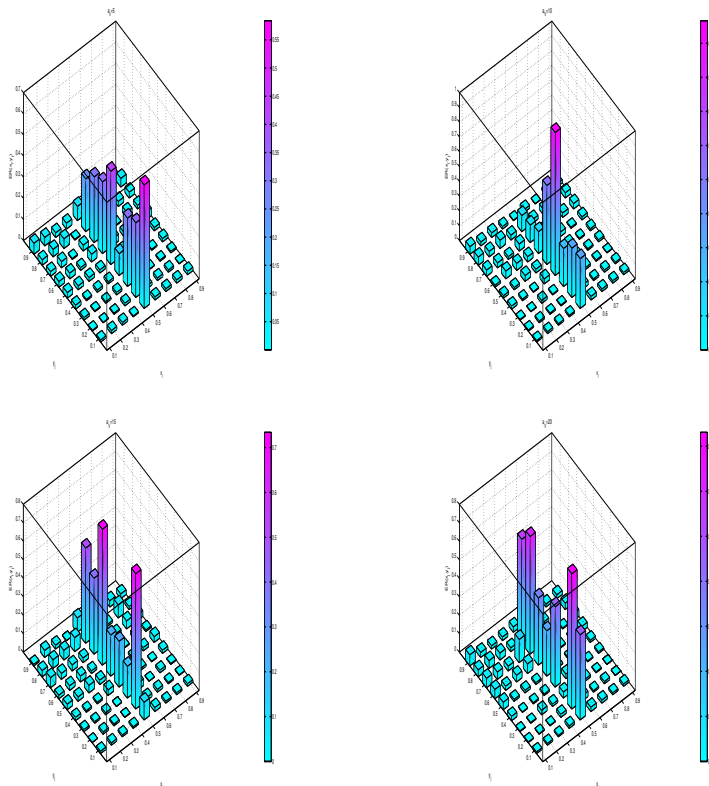
$a_V$	$ER_{\max}$	at point $(x_i, y_i)$	mean(ER)
5	0.0248	at (0.2;0.2)	0.0086
10	0.0182	at (0.1;0.1)	0.0055
15	0.0336	at (0.1;0.2)	0.0074
20	0.0214	at (0.1;0.3)	0.0076

**Fig. 3** BVP  $P_1$ : Empirical errors in the unit square when  $a_V = 5, 10, 15, 20$ **Table 3** BVP  $P_2$ : Maximum empirical error and error mean for different  $a_V$ 

$a_V$	$ER_{\max}$	at point $(x_i, y_i)$	mean(ER)
5	0.3250	at (0.5;0.1)	0.0497
10	0.6922	at (0.5;0.4)	0.0531
15	0.6208	at (0.5;0.6)	0.0569
20	0.7145	at (0.5;0.2)	0.0612

**Table 4** BVP  $P_2$ : 95% confidence intervals when empirical error is maximum

$a_V$	95% confidence interval	at point $(x_i, y_i)$
5	$[-0.025899; 0.09089]$	at $(0.5; 0.1)$
10	$[-0.027408; 0.16584]$	at $(0.5; 0.4)$
15	$[-0.011347; 0.13551]$	at $(0.5; 0.6)$
20	$[-0.001648; 0.14454]$	at $(0.5; 0.2)$

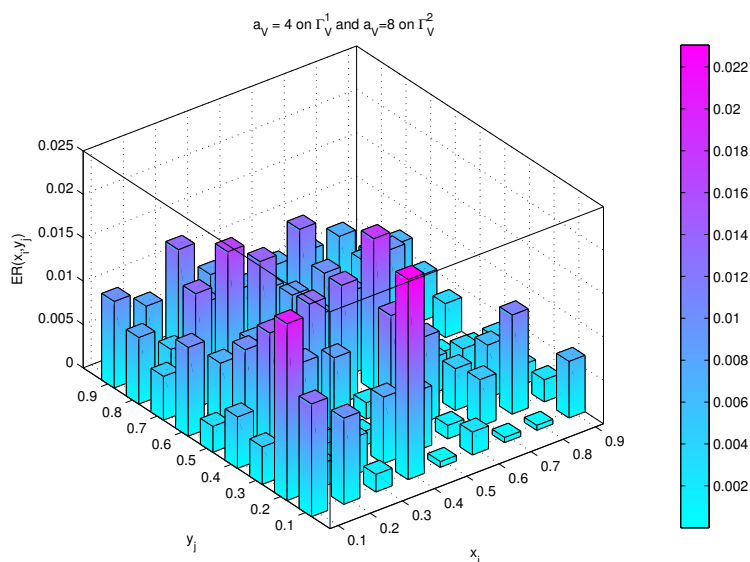
**Fig. 4** BVP  $P_2$ : Empirical errors in the unit square when  $a_V = 5, 10, 15, 20$ 

Let us finally consider the BVP  $P_1$  with a coefficient  $a_V$  different on each part of  $\Gamma_V$ ; the results are analogous as for instance:

$$a_V = \begin{cases} 4 & \text{on } \Gamma_V^1 = ]0, 1[ \times \{0\} \\ 8 & \text{on } \Gamma_V^2 = ]0, 1[ \times \{1\} \end{cases}$$

with the following data:

1. Number of simulated random walks:  $NT = 1 \times 10^4$ , i.e.  $2NT = 2 \times 10^4$  by means of antithetic variables



**Fig. 5** Empirical error when  $a_V$  is different on each part of  $\Gamma_V$

2. Stepsize of each random walk:  $h = 0.01$

The empirical errors  $ER_{ij}$  for  $a_V$  non constant are given in Figure 5.

#### 4.3 Wentzell-Dirichlet mixed BVP in quadrant of a ring

Let us consider problem (4) in  $G = \{(x, y) \in \mathbb{R}^2 \mid 1 < x^2 + y^2 < 9, x > 0, y > 0\}$  with the following data:

$$f \equiv -2 \text{ in } G$$

$$\Gamma_D = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 1, x \geq 0, y \geq 0\} \\ \cup \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 9, x \geq 0, y \geq 0\}$$

$$g_D \equiv 4 \text{ on } \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 1, x \geq 0, y \geq 0\}$$

$$g_D \equiv 9 \text{ on } \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 9, x \geq 0, y \geq 0\}$$

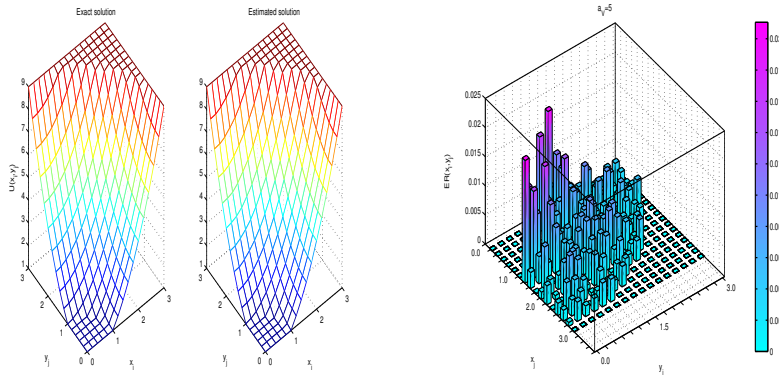
$$\Gamma_V = ([1, 3[ \times \{0\}) \cup (\{0\} \times ]1, 3])$$

$$g_V^r \equiv a_V \text{ on } \Gamma_V$$

$$g_V^v \equiv 0 \text{ on } \Gamma_V$$

such that this Wentzell-Dirichlet BVP admits a unique solution  $u$  written in the form:

$$u(x, y) = x^2 + y^2.$$



**Fig. 6** Exact and estimated solutions — Empirical error on quadrant of a ring

Let us consider the points  $Q_{ij} = Q(x_i, y_j) \in G$ , where  $x_i = 0.2 \times i$ ,  $0 \leq i \leq 15$ ,  $y_j = 0.2 \times j$ ,  $0 \leq j \leq 15$ , and  $1 < x_i^2 + y_j^2 < 9$ , i.e. a total number of 163 points in  $G$ .

The estimated solution  $u_c(x_i, y_j)$  and empirical error  $ER_{ij}$  when the boundary diffusion coefficient  $a_V$  equals to 5, are obtained with the following data:

1. Number of simulated random walks:  $NT = 10^4$ , i.e.  $2NT = 2 \times 10^4$  by means of antithetic variables
2. Stepsize of each random walk:  $h = 0.01$

and are given in Figure 6.

*Remark 3* When the number of realizations is  $NT = 10^4$ , the average CPU time used by the MATLAB® application implemented with a processor Intel i7 2.67 GHz (6.9 operations per second) for the numerical resolution of the BVP  $P_2$  in the unit square, equals to 160 seconds when the results are displayed at each point, and 97 second per point without displaying.

The results can be improved by using more realizations and smaller stepsize  $h$ , but this increases CPU time involved. Let us note that the reflections increase the CPU time involved, in particular when the initial point of the random walk is near one part of the boundary  $I_V$ .

## 5 Concluding remarks

In the present paper, we have presented stochastic method for the numerical approximation of some boundary value problems with Wentzell's boundary part and superabundant data on this part. The representations of solution are deduced from the application of Itô's formula even when the boundary data are non smooth. These probabilistic interpretations have given some easily implementable algorithms: they consist in the simulation of diffused-reflected random walks in order to generate samples from a distribution having a mean equal to the solution of the Wentzell BVP considered. This algorithm do not require to store in memory any mesh of the region

$G$ , nor deal with the corresponding numbering-lists. Programming is short, easy to check step by step.

As for the classical Monte Carlo schemes, this stochastic method admits an expected rate of convergence of about  $1/\sqrt{NT}$ . Relative error and empirical variance can be computed. The variance reduction techniques as antithetic variates can be applied. The essential properties of Monte Carlo methods are maintained; on the one hand, this stochastic method of the solution approximation does not depend on the choice of the point, on the other hand, their implementations on a parallel computer are intrinsically possible.

The development of the stochastic methods by the means of an integral representation makes possible not only the solution of these systems but extensions to more general models with general linear elliptic or parabolic operators and with wide classes of boundary conditions.

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