

# FIRST EXIT TIMES PROBABILITY FOR MULTIDIMENSIONAL DIFFUSIONS: A PDE-BASED APPROACH

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**ABSTRACT.** First exit times distribution for multidimensional processes are key quantities in many area of risk management and option pricing. The aim of this paper is to provide a flexible, fast and accurate algorithm for computing the probability of the first exit time from a bounded domain for multidimensional diffusions. First, we show that the probability distribution of this stopping time is the unique (weak) solution of a parabolic initial and boundary value problem. Then, we describe the algorithm which is based on a combination of the sparse tensor product Finite Element spaces and an hp-discontinuous Galerkin method. We illustrate our approach by several examples. We also compare the numerical results to classical Monte-Carlo methods.

## 1. Introduction

First exit times distribution for multidimensional random processes are key quantities in many fields of sciences, such as mathematical physics, neurology, and also in mathematical finance. For instance, in the latter case, it is required for the pricing of some path-dependent options and for estimating the risk of default in the structural approach. Unfortunately, closed form solutions to this problem are not attainable except in few specific cases. In this paper, we suggest a flexible and efficient numerical scheme based on PDE techniques, for computing the distribution of the first exit time from a bounded domain for multidimensional diffusions. We start by showing that the probability distribution of this stopping time can be represented as the unique weak solution of the backward Kolmogorov equation associated to the process subject to appropriate initial and boundaries conditions. It is well-known that the strong solution of an initial boundary value problem admits a probabilistic representation due to the Feynman-Kac formula, see Freidlin [3, Theorem 2.3]. Unfortunately, because of the incompatibility of the initial and boundary conditions in our problem, we can not get such solution. To overcome this difficulty, we derive a variational formulation of the problem which will be also used for the numerical approach. Under some smoothness conditions on the coefficients of the diffusion and by using well known results on variational problems, we derive the existence and uniqueness of a weak solution. At a second stage due to smoothness of the free terms, we deduce that the solution is locally strong, thus admits a Feynman-Kac type representation. We conclude by a uniqueness and a limiting argument that the first exit time probability is in fact the weak solution of the variational form of the Kolmogorov equation. For solving this problem numerically straightforward application of standard schemes fails due to the so-called ‘curse

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of dimension': the number of degrees of freedom on a tensor product Finite Element mesh of width  $h$  in dimension  $d$  grows like  $O(h^{-d})$  as  $h \rightarrow 0$ . This can be avoided by using sparse tensor product spaces and an  $hp$ -discontinuous Galerkin (DG) time stepping procedure as in [8]. The resulting algorithm requires  $O(h^{-1} |\log h|^{2d+6})$  operations. Compared to classical simulation techniques where Monte Carlo simulations are combined with discretization schemes for SDE's, our approach turns out to be more accurate and faster even for high-dimensional problems. It is also more flexible in the sense that we do not need the knowledge of the transition densities of the process unlike for simulation algorithms developed recently, see e.g. Mannella [6]. Moreover, the PDE approach provides the density at no additional costs using the ansatz functions for the time discretization and computes the distribution of the stopping time for any starting point of the diffusion in only one run.

The outline of the paper is as follows. We start by describing the set up of the problem and fix the notation. In Section 2, we show that, under some regularity conditions on the coefficients of the diffusions and on the domain, the exit probability is the unique weak solution of the backward Kolmogorov equations subject to specific initial and boundary conditions. Section 3 is devoted to the description of the numerical algorithm which includes sparse tensor product Finite Element spaces and an  $hp$ -discontinuous Galerkin time integration. Finally, we give numerical results and compare the PDE approach with classical Monte Carlo methods.

**1.1. The First Exit Time Problem.** Let  $(\Omega, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$  be a filtered probability space and  $\mathbf{X} := (X^1, \dots, X^d)$ , with  $\mathbf{x} := (x_1, \dots, x_d)$ , be the solution to the following system of stochastic differential equations

$$(1.1) \quad dX_t^i = b_i(\mathbf{X}_t) dt + \sum_{j=1}^d \sigma_{ij}(\mathbf{X}_t) dW_t^j, \quad X_0^i = x_i \in \mathbb{R}$$

where  $W := (W^1, \dots, W^d)^T$  is a  $d$ -dimensional standard Brownian motion with  $d \geq 1$  and the coefficients  $b_i$  and  $\sigma_{ij}$  are smooth enough, see e.g. Stroock and Varadhan [9]. We denote the infinitesimal generator of  $\mathbf{X}$  by  $\mathcal{G}$  which has the form

$$(1.2) \quad \mathcal{G}f(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^d \sum_{j=1}^d a_{ij}(\mathbf{x}) \frac{\partial^2 f(\mathbf{x})}{\partial x_i \partial x_j} + \sum_{i=1}^d b_i(\mathbf{x}) \frac{\partial f(\mathbf{x})}{\partial x_i}$$

where  $a = \sigma \sigma^\top$  and  $f \in C_K^2(\mathbb{R}^d)$ , the space of twice continuously differentiable functions on  $\mathbb{R}^d$  with compact support.

Let  $A$  be an open bounded Borel subset of  $\mathbb{R}^d$  with boundary denoted by  $\partial A$  and define the stopping time

$$(1.3) \quad \tau_A = \inf\{u \geq 0; \mathbf{X}_u \notin A\}.$$

This is the first exit time of  $\mathbf{X}$  from the domain  $A$  where we assume that  $\partial A$  is smooth enough. Let us denote by  $\mathbb{Q}(t, \mathbf{x})$  the probability that  $\mathbf{X}$  starting from  $\mathbf{x}$  did not exit the domain  $A$  before  $t$ , i.e.

$$(1.4) \quad \mathbb{Q}(t, \mathbf{x}) = 1 - \mathbb{P}_{\mathbf{x}}(\tau_A < t).$$

Formally,  $\mathbb{Q}$  coincides with the solution of the following backward Kolmogorov equation associated to the process  $\mathbf{X}$

$$(1.5a) \quad \frac{\partial u}{\partial t}(t, \mathbf{x}) = \mathcal{G}u(t, \mathbf{x}) \quad \text{on } (t, \mathbf{x}) \in \mathbb{R}^+ \times A$$

$$(1.5b) \quad u(0, \mathbf{x}) = 1, \quad \mathbf{x} \in A$$

$$(1.5c) \quad u(t, \mathbf{x}) = 0, \quad \mathbf{x} \in \partial A, t > 0.$$

**1.2. Notation.** Throughout the paper, we use the following notations. Let  $V$  and  $H$  separable Hilbert spaces with dense injection  $V \xhookrightarrow{d} H$  and norms  $\|\cdot\|_V$  and  $\|\cdot\|_H$ , respectively. Denoting by  $(\cdot, \cdot)_H$  the scalar product on  $H$  and identifying  $H$  with  $H^*$ , the antidual of  $H$ , we get the Gelfand triple

$$V \xhookrightarrow{d} H \cong H^* \xhookrightarrow{d} V^*.$$

We denote by  $(\cdot, \cdot)_{V^*, V}$  the usual duality pairing in  $V^* \times V$  and by  $\|\cdot\|_{V^*}$  the norm in  $V^*$ . Next, for any  $T > 0$ , we consider the spaces

$$\mathcal{V} = L^2(0, T; V) \quad \text{and} \quad \mathcal{H} = L^2(0, T; H)$$

where if  $K$  is a Hilbert space,  $L^2(0, T; K)$  denotes class of measurable functions  $f : (0, T) \rightarrow K$  for the Lebesgue measure such that  $\int_0^T \|f(t)\|_K^2 dt < \infty$ . Then, we have

$$\mathcal{V}^* = L^2(0, T; V^*).$$

Furthermore,  $H_0^1(A)$  is defined by  $H_0^1(A) = \{v \in H^1(A); v|_{\partial A} = 0\}$  with the norm

$$\|v\|_{H_0^1(A)}^2 = \sum_{i=1}^d \left\| \frac{\partial v}{\partial x_i} \right\|_{L^2(A)}^2 + \|v\|_{L^2(A)}^2.$$

For any  $T > 0$ , we denote by  $Q_T$  the cylinder  $A \times (0, T)$  and introduce the Hölder spaces  $\mathcal{H}^{l, l/2}(Q_T)$ , for a nonintegral positive number  $l$ .  $\mathcal{H}^{l, l/2}(Q_T)$  is the Banach space of functions  $u(x, t)$  that are continuous in  $Q_T$ , together with all derivatives of the form  $\frac{\partial^r}{\partial t^r} \frac{\partial^s}{\partial x^s}$  for  $2r + s < l$  and have a finite norm

$$\|u\|_{Q_T}^{(l)} = \langle u \rangle_{Q_T}^{(l)} + \sum_{j=0}^{[l]} \langle u \rangle_{Q_T}^{(j)}$$

where

$$\langle u \rangle_{Q_T}^{(0)} = \max_{Q_T} |u|, \quad \|u\|_{Q_T}^{(l)} = \sum_{2r+s=l} \left| \frac{\partial^r u}{\partial t^r} \frac{\partial^s u}{\partial x^s} \right|_{Q_T}^{(0)}.$$

## 2. First exit time probability as the weak solution of the Kolomogorov equation

We provide sufficient conditions on the coefficients of the diffusion and on the boundary of the domain  $A$  which ensure that the exit probability  $\mathbb{Q}$  is the (weak) solution of the parabolic problem (1.5). Although it seems to be a classical result, to the best of our knowledge, we did not find any rigorous proof of such a representation of the first exit time probability.

**2.1. The variational formulation of the backward Kolomogorov equation.** In this part, we recall briefly the variational formulation of abstract parabolic problems and provide the assumptions under which existence and uniqueness of the weak solution are ensured. Consider for  $F \in \mathcal{V}^*$  and  $u_0 \in H$  the abstract parabolic problem

$$(2.1a) \quad \frac{d}{dt} (u(t, \cdot), v)_V + g(u(t, \cdot), v) = (F, v)_{V^*, V} \quad \forall v \in V, \quad 0 < t \leq T,$$

$$(2.1b) \quad (u(0, \cdot), v)_H = (u_0, v)_H \quad \forall v \in V.$$

The derivative  $\frac{d}{dt}$  is understood in the weak sense. We are now ready to state the following general result for the existence and uniqueness of a weak solution of the parabolic problem, see [5, Theorem 4.4.1 and Remark 4.4.3]

**Proposition 2.1.** *Assume that the bilinear form  $g(\cdot, \cdot)$  in (2.1a) is*

(1) *continuous, i.e. there exists a constant  $c > 0$  such that*

$$(2.2) \quad \|g(u, v)\|_H \leq c \|u\|_V \|v\|_V \quad \forall u, v \in V,$$

(2) *coercive on  $V$ , i.e. there exist positive constants  $\lambda$  and  $\alpha$  such that*

$$(2.3) \quad g(v, v) + \lambda \|v\|_H^2 \geq \alpha \|v\|_V^2 \quad \forall v \in V.$$

*Then for any  $F \in \mathcal{V}^*$ , there exists a unique  $u \in \mathcal{V}$  solution of (2.1a)–(2.1b).*

**Remark 2.2.** Note that (2.1a) implies that  $\frac{d}{dt}u \in \mathcal{V}^*$ , so that

$$(2.4) \quad u \in C^0([0, T], H) \cap H^1(0, T; V^*).$$

We make the following assumptions.

**Assumption 2.3.** (1) *The coefficients  $\sigma_{i,j}$ ,  $1 \leq i, j \leq d$ , in (1.1) are  $(k-1)$ -times continuously differentiable on  $A$ .*

(2) *The coefficients  $b_i$ ,  $1 \leq i \leq d$ , in (1.2) are  $(k-1)$ -times continuously differentiable on  $A$ .*

(3) *There exists a constant  $\alpha > 0$  such that*

$$(2.5) \quad \sum_{i=1}^d \sum_{j=1}^d a_{i,j}(\mathbf{x}) \xi_i \xi_j \geq \alpha \sum_{i=1}^d \xi_i^2, \quad \forall \xi_i \in \mathbb{R}, \mathbf{x} \in A.$$

(4)  *$\partial A$  is piecewise smooth (as defined in Ladyzenskaja et al. [4]).*

We take  $H = L^2(A)$  and  $V = H_0^1(A)$  so that  $V^* = H^{-1}(A)$  and specify the bilinear form  $g(\cdot, \cdot)$  defined on  $H_0^1(A) \times H_0^1(A)$  by

$$g(u, v) = \frac{1}{2} (a \nabla u, \nabla v)_{L^2(A)} - ((b - \operatorname{div} a) \nabla u, v)_{L^2(A)}.$$

Now the Kolmogorov variational problem reads

$$(2.6a) \quad \frac{d}{dt} (u(t, \cdot), v)_{L^2(A)} + g(u(t, \cdot), v) = 0 \quad \forall v \in H_0^1(A),$$

$$(2.6b) \quad u(0, \cdot) = 1.$$

**Theorem 2.4.** *Under Assumptions 2.3 the bilinear form  $g(.,.)$  satisfies the continuity and coerciveness conditions. As a consequence, the problem (2.6a)–(2.6b) admits a unique variational solution*

$$(2.7) \quad u \in L^2(0, T; H_0^1(A)) \cap C^0([0, T]; L^2(A)) \cap H^1(0, T; H^{-1}(A)).$$

**Proof.** Let  $u \in H_0^1(A)$ , then we have

$$g(u, u) = \frac{1}{2} (a \nabla u, \nabla u)_{L^2(A)} - ((b - \nabla a) \nabla u, u)_{L^2(A)}.$$

By using Cauchy inequality, we obtain, for any  $c_2 > 0$ ,

$$\left( b_j \frac{\partial u}{\partial x_j}, u \right)_{L^2(A)} \leq \|b_j\|_{L^\infty(A)} \left( c_2 \|u\|_{L^2(A)}^2 + \frac{1}{4c_2} \left\| \frac{\partial u}{\partial x_j} \right\|_{L^2(A)}^2 \right).$$

Together with (2.5), we get

$$g(u, u) \geq \frac{\alpha}{2} \|\nabla u\|_{L^2(A)} - \|b - \nabla a\|_{L^\infty(A)} \left( c_2 \|u\|_{L^2(A)}^2 + \frac{1}{4c_2} \|\nabla u\|_{L^2(A)}^2 \right).$$

We conclude by choosing  $c_2 \geq \frac{\|b - \nabla a\|_{L^\infty(A)}}{2\alpha}$  to get the coerciveness conditions (2.3) and obtain the Theorem from Proposition 2.1.  $\square$

**Remark 2.5.** By integration by parts, one observes that  $u$  satisfies (1.5) in the sense of distribution in  $Q_T$ , (1.5b) holds in the topology of  $L^2(A)$  and the boundary condition (1.5c) is contained in the fact that  $u \in L^2(0, T; H_0^1(A))$  and  $A$  is regular.

**2.2. Regularity of the weak solution.** Thanks to the smoothness of the free terms of the problems and the regularity of  $A$ , the weak solution has some regularity. We have the following classical (local) regularity result, see e.g. Ladyzenskaja et al. [4, Theorem III.12.1].

**Proposition 2.6.** *Let Assumption 2.3 holds and fix  $\alpha$  such that  $[\alpha] = 1$ . Then, the unique solution of the variational problem (2.6a)–(2.6b) belongs to*

$$(2.8) \quad u \in \mathcal{H}^{2+\alpha, 1+\alpha/2}(Q_T) \cap C^0([0, T] \times A).$$

Moreover, for any  $t_0 > 0$ ,

$$(2.9) \quad u \in C^0([t_0, T]; C^2(A) \cap C^0(\bar{A})).$$

**2.3. The probabilistic representation.** We end up this section with the following result.

**Theorem 2.7.** *Let Assumption 2.3 holds. Then, the unique weak solution  $u(t, \mathbf{x})$  of the variational Kolmogorov equation (2.6a)–(2.6b), belongs to*

$$(2.10) \quad \mathcal{H}^{2+\alpha, 1+\alpha/2}(Q_T) \cap C^0([0, T] \times A)$$

and coincides with  $\mathbb{Q}(t, \mathbf{x}) = 1 - \mathbb{P}_{\mathbf{x}}(\tau_A < t)$  for all  $x \in \bar{A}$ ,  $0 < t \leq T$ .

**Proof.** Let  $u$  be the weak solution of (2.6a)–(2.6b). From Proposition 2.6, we have, for any  $t_0 > 0$ ,  $u \in C^0([t_0, T]; C^2(A) \cap C^0(\bar{A}))$ . We deduce, from [3, Theorem II.2.3] and Remark 2.5, that  $u$  has the following probabilistic representation, setting  $\tau_A^t = \tau_A \wedge t$ , for any  $t > 0$  and any  $\mathbf{x} \in A$ ,

$$(2.11) \quad u(t, \mathbf{x}) = \mathbb{E}_{\mathbf{x}} \left[ \mathbb{I}_{\{\tau_A^t = t\}} \right] = \mathbb{Q}(t, \mathbf{x}).$$

That is, we have, for any  $t > 0$  and  $\mathbf{x} \in \bar{A}$ ,  $u(t, \mathbf{x}) = \mathbb{Q}(t, \mathbf{x})$ . From (2.8), we know that  $u \in C^0([0, T] \times A)$  which implies that  $\lim_{t \searrow 0} u(t, \mathbf{x}) = 1$  for any  $\mathbf{x} \in A$ . Moreover, by uniqueness of both the probabilistic representation and the solution of (1.5)-(1.5b), we get, for any  $\mathbf{x} \in A$ , that

$$\lim_{t \searrow 0} \mathbb{Q}(t, \mathbf{x}) = \lim_{t \searrow 0} u(t, \mathbf{x}) = 1.$$

The proof of the Theorem is then completed by observing that  $u$  and  $\mathbb{Q}$  coincides on  $\{t = 0\} \times A \cup \{t > 0\} \times \bar{A}$ .  $\square$

**Remark 2.8.** We point out that we could actually consider more general diffusions and/or weaken the assumption on the boundary of the domain  $A$ . We could for instance consider time-dependent coefficients for the diffusion (1.1). In this case, the Assumption 2.3 should hold uniformly in time.

### 3. Numerical Algorithm

As mentioned in the Introduction, a straightforward application of standard numerical schemes for solving (1.5) fails due to the so-called ‘curse of dimension’: the number of degrees of freedom on a tensor product Finite Element mesh of width  $h$  in dimension  $d$  grows like  $O(h^{-d})$  as  $h \rightarrow 0$ . Therefore, Monte Carlo methods are mostly used where the error decreases like  $O(M^{-1/2})$  if one uses  $M$  simulations. This holds for any  $d \geq 1$ , but only in a probabilistic sense. We use the algorithm described in Petersdorff and Schwab [8] which provides an error of  $O(N^{-p})$  where  $p$  is the degree of the finite elements which can be any integer  $\geq 1$ . The method is based on the following two observations.

(i) To reduce the number of degrees of freedom in high dimensions, so-called sparse tensor product Finite Element spaces are used. Their number of degrees of freedom grow like  $O(h^{-1} |\log h|^{d-1})$  as  $h \rightarrow 0$ , instead of  $O(h^{-d})$  for the full tensor product spaces. At the same time, the approximation rate in  $H^1(A)$  for elements of degree  $p \geq 1$  and smooth functions is  $O(h^p)$ , the same as for full tensor product spaces. This result requires more regularity than  $H^{p+1}(A)$  for the approximated function, and the amount of extra regularity increases with  $d$ . In the problem mentioned above, the initial data  $u_0$  is incompatible with the boundary conditions. However, the solution operator  $E(t)$  of the parabolic problem is an analytic semigroup and increases the smoothness of the solution  $u(\cdot, t)$  for  $t > 0$ . This parabolic smoothing effect suffices for optimal convergence of sparse space discretization at  $T > 0$  for any  $d$ , even for initial data that are just in  $L^2(A)$ .

(ii) Even with a sparse space discretization the number  $\hat{N}_L$  of spatial degrees of freedom is substantial if  $d$  is large. Reducing the number of time steps (and thus, the number of spatial problems to be solved) to pass from  $t = 0$  to the final time  $T$  is therefore essential. Time analyticity of  $E(t)$  implies analytic time regularity of the solution  $u(t)$  for  $t > 0$ , but not uniformly in  $(0, T)$ . This allows to construct  $hp$ -discontinuous Galerkin time-stepping schemes with exponential convergence in the number of spatial problems.

**3.1. Sparse Tensor Product Spaces.** In the interval  $I = (0, 1)$ , we define the mesh  $\mathcal{T}^\ell$  given by the nodes  $j2^{-\ell}$ ,  $j = 0, \dots, 2^\ell$ , with the mesh width  $h_\ell = 2^{-\ell}$ . We define  $\mathcal{V}^\ell$  as the space of piecewise polynomials of degree  $p \geq 1$  on the mesh  $\mathcal{T}^\ell$  which are in  $C^{p'-1}([0, 1])$  with  $1 \leq p' \leq p$  and vanish at the endpoints  $0, 1$ . We write  $N^\ell = \dim \mathcal{V}^\ell$ ,  $M^\ell := N^\ell - N^{\ell-1}$ ,  $N^{-1} := 0$ ; then

$N^\ell = O(2^\ell)$ ,  $\ell = 0, 1, 2, \dots$ . We employ a wavelet basis  $\psi_j^\ell$ ,  $j = 1, \dots, M^\ell$ ,  $\ell = 0, 1, 2, \dots$  of  $\mathcal{V}^\ell$  with the properties

$$(3.1) \quad \mathcal{V}^\ell = \text{span}\{\psi_j^\ell \mid 0 \leq \ell \leq L; 1 \leq j \leq M^\ell\} \quad \text{and} \quad \text{diam}(\text{supp } \psi_j^\ell) \leq C 2^{-\ell}.$$

Any function  $v \in \mathcal{V}^L$  has the representation

$$(3.2) \quad v = \sum_{\ell=0}^L \sum_{j=1}^{M^\ell} v_j^\ell \psi_j^\ell$$

with  $v_j^\ell = (v, \tilde{\psi}_j^\ell)$  where  $\tilde{\psi}_j^\ell$  are the so-called dual wavelets. For  $v \in H_0^1(I)$  one obtains the series

$$(3.3) \quad v = \sum_{\ell=0}^{\infty} \sum_{j=1}^{M^\ell} v_j^\ell \psi_j^\ell$$

which converges in  $L^2(I)$  and in  $H_0^1(I)$ .

For  $v \in L^2(I)$  we can define a projection  $P_L : L^2(I) \rightarrow \mathcal{V}^L$  by truncating (3.3)

$$(3.4) \quad P_L v := \sum_{\ell=0}^L \sum_{j=1}^{M^\ell} v_j^\ell \psi_j^\ell, \quad P_{-1} := 0.$$

The increment or detail spaces  $\mathcal{W}^\ell$  are defined by

$$(3.5) \quad \begin{cases} \mathcal{W}^\ell := \text{span}\{\psi_j^\ell : 1 \leq j \leq M^\ell\}, & \ell = 1, 2, 3, \dots \\ \mathcal{W}^0 := \mathcal{V}^0. \end{cases}$$

Then

$$(3.6) \quad \mathcal{V}^\ell = \mathcal{V}^{\ell-1} \oplus \mathcal{W}^\ell \text{ for } \ell \geq 1, \quad \text{and} \quad \mathcal{V}^\ell = \mathcal{W}^0 \oplus \dots \oplus \mathcal{W}^\ell, \ell \geq 0.$$

and  $Q_\ell := P_\ell - P_{\ell-1}$  is a projection from  $L^2(I)$  to  $\mathcal{W}^\ell$ .

In  $I^d = (0, 1)^d$ ,  $d > 1$  we define the subspace  $V^L$  as the tensor product of the one-dimensional spaces

$$(3.7) \quad V^L := \mathcal{V}^L \otimes \dots \otimes \mathcal{V}^L$$

which can be written using (3.6) as

$$(3.8) \quad V^L = \sum_{0 \leq \ell_i \leq L} \mathcal{W}^{\ell_1} \otimes \dots \otimes \mathcal{W}^{\ell_d}.$$

The space  $V^L$  has  $O(2^{Ld})$  degrees of freedom and is too costly if  $d$  is large. We shall use the sparse tensor product space

$$(3.9) \quad \begin{aligned} \widehat{V}^L &:= \text{span} \left\{ \psi_{j_1}^{\ell_1}(x_1) \dots \psi_{j_d}^{\ell_d}(x_d) \mid 1 \leq j_i \leq M^{\ell_i}, \ell_1 + \dots + \ell_d \leq L \right\} \\ &= \sum_{0 \leq \ell_1 + \dots + \ell_d \leq L} \mathcal{W}^{\ell_1} \otimes \dots \otimes \mathcal{W}^{\ell_d}. \end{aligned}$$

As  $L \rightarrow \infty$ , we have  $N_L := \dim(V^L) = O(2^{dL})$ , and  $\widehat{N}_L := \dim(\widehat{V}^L) = O(L^{d-1} 2^L)$ , i.e. the spaces  $\widehat{V}^L$  have considerably smaller dimension than  $V^L$ . On the other hand, they do have

similar approximation properties as  $V^L$ , provided the function to be approximated is sufficiently smooth.

**3.2. Discontinuous Galerkin Time Stepping.** We first analyze the time discretization of the parabolic problem (1.5)

$$\begin{aligned} u'(t) - \mathcal{G}u(t) &= 0 & t \in (0, T], \\ u(0) &= u_0 \end{aligned}$$

with  $u_0 = 1$ .

Let  $\mathcal{M}$  be a partition of  $(0, T)$  into  $M(\mathcal{M})$  timesteps  $\{I_m\}_{m=1}^M$ ,  $I_m = (t_{m-1}, t_m)$ ,  $1 \leq m \leq M$ , of size  $k_m = t_m - t_{m-1}$ . Define the one-sided limits of  $u \in \mathcal{H}$  (or  $\mathcal{V}$ ) as

$$(3.10) \quad \begin{aligned} u_m^+ &:= \lim_{s \rightarrow 0^+} u(t_m + s), & 0 \leq m \leq M-1, \\ u_m^- &:= \lim_{s \rightarrow 0^+} u(t_m - s), & 1 \leq m \leq M \end{aligned}$$

and  $[u]_m := u_m^+ - u_m^-$ ,  $1 \leq m \leq M-1$ .

The weak solution  $u \in L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*)$  of (1.5) satisfies

$$B_{\text{DG}}(u, v) = (u_0, v_0^+)$$

for all

$$v \in C_b(\mathcal{M}; \mathcal{V}) := \{u : (0, T) \rightarrow \mathcal{V} : u|_{I_m} \in C^0(\bar{I}_m; \mathcal{V}), I_m \in \mathcal{M}\}$$

where

$$\begin{aligned} B_{\text{DG}}(u, v) &:= \sum_{m=1}^M \int_{I_m} \{(u', v)_{\mathcal{V}^* \times \mathcal{V}} + g(u, v)\} dt \\ &\quad + (u_0^+, v_0^+)_{\mathcal{H}} + \sum_{m=2}^M ([u]_{m-1}, v_{m-1}^+)_{\mathcal{H}}. \end{aligned}$$

With time step  $k_m$  we associate an order  $r_m \geq 0$ , and define the semidiscrete space

$$\mathcal{S}^{\vec{r}}(\mathcal{M}; \mathcal{V}) = \{u : (0, T) \rightarrow \mathcal{V} : u|_{I_m} \in \mathcal{P}^{r_m}(I_m; \mathcal{V}), 1 \leq m \leq M\}$$

with the order vector  $\vec{r} := (r_1, \dots, r_M)$ . The number of unknown coefficient functions in  $\mathcal{V}$  of  $u \in \mathcal{S}^{\vec{r}}(\mathcal{M}; \mathcal{V}) := \mathcal{S}^{\vec{r}}(\mathcal{M}) \otimes \mathcal{V}$  is

$$\dim(\mathcal{S}^{\vec{r}}(\mathcal{M})) = \sum_{m=1}^M (r_m + 1).$$

For simplicity we will consider uniform orders, i.e.  $r_m = r$  for all  $m$  and write  $\mathcal{S}^{\vec{r}} = \mathcal{S}^r(\mathcal{M}; \mathcal{V})$ . It is shown in [8] that for geometric meshes  $\mathcal{M}$  the approximation error decreases exponentially in  $N = \dim(\mathcal{S}^r(\mathcal{M}))$ . A mesh  $\{I_m\}_{m=1}^M$  in  $(0, T)$  is geometric with  $M$  time steps  $I_m = (t_{m-1}, t_m)$ ,  $m = 1, \dots, M$ , and grading factor  $\eta \in (0, 1)$ , if

$$t_0 = 0, \quad t_m = T\eta^{M-m}, \quad 1 \leq m \leq M.$$

3.2.1. *Fully discrete problem.* We now also discretize the space  $A = (0, 1)^d$  with the sparse grid subspace  $\widehat{V}^L$  of  $V$  of meshwidth  $h = 2^{-L}$ ,  $L > 0$ . The discontinuous Galerkin time-stepping scheme is given by:

Find  $\widehat{U}^L \in \mathcal{S}^r(\mathcal{M}; \widehat{V}^L)$  such that

$$B_{\text{DG}}(\widehat{U}^L, \widehat{W}) = (u_0, \widehat{W}_0^+) \quad \forall \widehat{W} \in \mathcal{S}^r(\mathcal{M}; \widehat{V}^L).$$

In each of the  $M$  time steps amounts to the solution of a linear system of size

$$(3.11) \quad (r+1)\widehat{N}_L = (r+1)O(h^{-1} |\log h|^{d-1})$$

which depends on the time step  $k$  and  $h$  and which we now derive.

Let  $\mathcal{Q} := \mathcal{P}_r(I_m, \widehat{V}^L)$ , equipped with the norm of  $L^2([t_{m-1}, t_m]) \otimes V$ . In time step  $m$  of the algorithm we have to determine  $\widehat{U}_m^L := \widehat{U}^L|_{I_m} \in \mathcal{Q}$  which satisfies, for all  $W \in \mathcal{Q}$ ,

$$(3.12) \quad \int_{t_{m-1}}^{t_m} \left[ \left( (\widehat{U}_m^L)' , W \right) + g(\widehat{U}_m^L, W) \right] dt + \left( \widehat{U}_m^L(t_{m-1}), W(t_{m-1}) \right) = \left( \widehat{U}_{m-1}^L(t_{m-1}), W(t_{m-1}) \right)$$

where the expression  $\widehat{U}_0^L(t_0)$  is defined to mean the initial value  $\widehat{u}_0^L$ .

Let  $\{\phi\}_{j=0}^{r_m}$  be a basis of the polynomial space  $\mathcal{P}_{r_m}(-1, 1)$ . Then, the time shape functions on time interval  $I_m$  are given by  $\phi_j \circ F_m^{-1}$  where the mapping  $F_m: (-1, 1) \rightarrow I_m$  is given by

$$t = F_m(\tau) = \frac{1}{2}(t_{m-1} + t_m) + \frac{1}{2}k_m\tau, \quad k_m = t_m - t_{m-1}, \quad \tau \in (-1, 1).$$

If we write  $\widehat{U}_m^L(x, t)$  and  $\widehat{W}$  in (3.12) as

$$(3.13) \quad \widehat{U}_m^L(x, t) = \sum_{j=0}^{r_m} \widehat{U}_{m,j}^L(x) (\phi_j \circ F_m^{-1})(t), \quad \widehat{W}(x, t) = \sum_{j=0}^{r_m} \widehat{W}_{m,j}^L(x) (\phi_j \circ F_m^{-1})(t),$$

the variational problem (3.12) has the following form:

Find  $(\widehat{U}_{m,j}^L)_{j=0}^r \in (\widehat{V}^L)^{r+1}$  such that for every  $(\widehat{W}_i)_{i=0}^r \in (\widehat{V}^L)^{r+1}$

$$(3.14) \quad \sum_{i,j=0}^r \left( C_{ij} \cdot (\widehat{U}_{m,j}^L, \widehat{W}_i)_H + \frac{k_m}{2} G_{ij} \cdot g(\widehat{U}_{m,j}^L, \widehat{W}_i) \right) = \sum_{i=0}^r f_{m,i}(\widehat{W}_i)$$

where

$$(3.15) \quad f_{m,i}(v) := \phi_i(-1) (\widehat{U}_{m-1}^L(t_{m-1}), v)_H$$

$$C_{ij} := \int_{-1}^1 \phi_j' \phi_i d\tau + \phi_j(-1) \phi_i(-1), \quad G_{ij} = \int_{-1}^1 \phi_j \phi_i d\tau.$$

Equation (3.14) is a linear system of size  $(r+1)\widehat{N}_L$  to be solved in each time step  $m = 1, \dots, M$ . We will drop the subscript  $m$  for sake of readability. Denoting by  $\mathbf{M}$  and  $\mathbf{S}$  the mass and stiffness matrix of  $\widehat{V}^L$  with respect to  $(\cdot, \cdot)_H$  and  $g(\cdot, \cdot)$ , respectively, (3.14) takes the matrix form

$$(3.16) \quad \mathbf{R}\vec{u} = \vec{f}, \quad \mathbf{R} = \mathbf{C} \otimes \mathbf{M} + \frac{k}{2} \mathbf{G} \otimes \mathbf{S}$$

where  $\vec{u}$  denotes the coefficient vector of  $\widehat{U}_m^L \in \mathcal{Q}$ .

3.2.2. *Derivation of a linear system.* From now on we will use temporal shape functions  $\phi_i(\tau) = (i + 1/2)^{1/2} L_i(\tau)$ . The system (3.16) of size  $(r + 1)\hat{N}_L$  can be reduced to solving  $r + 1$  linear systems of size  $\hat{N}_L$ . We use the Schur decomposition  $\mathbf{C} = \mathbf{Q}\mathbf{T}\mathbf{Q}^H$  with a unitary matrix  $\mathbf{Q}$  and an upper triangular matrix  $\mathbf{T}$  which has the eigenvalues  $\lambda_1, \dots, \lambda_{r+1}$  of  $\mathbf{C}$  on the diagonal. Multiplying (3.16) by  $\mathbf{Q}^H \otimes \mathbf{I}$  from the left gives

$$\left( \mathbf{T} \otimes \mathbf{M} + \frac{k}{2} \mathbf{I} \otimes \mathbf{S} \right) \vec{w} = \vec{g}$$

with

$$\vec{w} := (\mathbf{Q}^H \otimes \mathbf{I}) \vec{x}, \quad \vec{g} := (\mathbf{Q}^H \otimes \mathbf{I}) \vec{f}.$$

This system is block-upper-triangular. With  $\vec{w} = (\vec{w}_0, \dots, \vec{w}_r)$  we obtain the solution by solving

$$(3.17) \quad \left( \lambda_{j+1} \mathbf{M} + \frac{k}{2} \mathbf{S} \right) \vec{w}_j = \vec{s}_j \quad \text{for } j = r, r-1, \dots, 0$$

where

$$\vec{s}_j := \vec{g}_j - \sum_{l=j+1}^r \mathbf{T}_{j+1, l+1} \mathbf{M} \vec{w}_l.$$

For each DG time step, we have to solve the  $r + 1$  linear systems in (3.17). Each of these linear systems is of the same type as in the backward Euler method where the matrix is  $\mathbf{M} + k\mathbf{S}$ . Therefore, an implementation of the DG method is very similar to an implementation of the backward Euler method.

**Remark 3.1.** We could also apply other time-stepping schemes for the time discretization. But the hp-discontinuous Galerkin scheme uses the analytic time regularity of the solution  $u(t)$  for  $t > 0$ . Especially for incompatible or non-smooth initial data this is an advantage since the number of time points can be reduced using geometric meshes obtaining exponential convergence rates.

## 4. Numerical Results

We first make a complexity comparison between the Monte-Carlo method and the deterministic approach. Then, we show the outcomes of numerical experiments from both approaches in the one-dimensional case, by considering the first exit time of an interval by a Brownian motion with a linear drift, where analytic formulas are available. Results for the analogue multidimensional case are also presented. All computations are performed on a Dual-Core AMD Opteron(tm) Processor 2218 with 2.61GHz using MATLAB 7.1.

Complexity comparison. Let  $\tau > 0$  be a given tolerance. It is known that for the Monte-Carlo method the statistical error is given by  $O\left(M^{-\frac{1}{2}}\right)$  where  $M$  is the number of simulations. Additionally, we have to discretize the SDE in time. For the Euler-Maruyama discretization the weak error is  $O(k)$  where  $k$  the number of time steps. To keep both errors at tolerance  $\tau$  we have

$$M \geq \tau^{-2} \quad \text{and} \quad k \geq \tau^{-1}.$$

The corresponding work for one single point is

$$W_{\text{mc}} = O(M \cdot k) = O(\tau^{-3}).$$

For the finite element method with hp-discontinuous Galerkin time stepping the  $\mathcal{H}_1$ -error is  $O(N^{-p-\delta})$  where  $N$  is the number of points,  $p$  the degree of the finite elements and  $\delta = \frac{p}{(p+1)d-1}$  (see [8]). Therefore, we have

$$N \geq \tau^{-\frac{1}{p+\delta}}$$

and the corresponding work for  $N$  points is

$$W_{\text{det}} = O\left(N(\log N)^{2d+6}\right) = O\left(\tau^{-\frac{1}{p+\delta}} \left| \frac{1}{p+\delta} \log \tau \right|^{2d+6}\right).$$

The one-dimensional case. Let  $-\infty < a_1 < a_2 < +\infty$  and set  $A = (a_1, a_2)$ ,  $b(x) = b \in \mathbb{R}$  and  $\sigma(x) = \sigma > 0$ . Then, the density of the first exit time of  $X$ , the (scaled-)Brownian motion with a linear drift  $b$ , from  $A$  is well known to be, see e.g. [1],

$$\begin{aligned} & \frac{d}{dt} \mathbb{P}\{\tau_A < t\} \\ &= e^{-\sigma^2 t/2} \left( e^{b(a_1-x)} \text{ss}_t(a_2-x, a_2-a_1) + e^{b(a_2-x)} \text{ss}_t(x-a_1, a_2-a_1) \right) \end{aligned}$$

where the help function  $\text{ss}_t$  has the following series representation

$$\text{ss}_t(v, y) = \sum_{k=-\infty}^{\infty} \frac{y-v+2ky}{\sqrt{2\pi t^3}} e^{-\frac{(y-v+2ky)^2}{2t}}.$$

We compare a Monte-Carlo approach with the deterministic algorithm described above. For the simulation we discretize the stochastic process

$$\tilde{X}(t+dt) = \tilde{X}(t) + b dt + \sigma \sqrt{dt} \tilde{Z}$$

with  $\tilde{X}(0) = x_0$  and  $\tilde{Z} \sim N(0, 1)$ . The random numbers are generated by the MATLAB function `randn`. We choose  $dt = 5 \cdot 10^{-4}$ , a random sample of the size  $10^5$  and count the number of sample paths which exceed  $A$ . For  $x_0$  we choose 9 points in the interval  $A$  equally spaced and use the same random sequences for each point.

In the deterministic approach we discretize the space with  $L = 6$  levels. For the hp-discontinuous Galerkin time stepping we use  $\log(2^{L+1})$  time steps with increasing polynomial degree  $r_m = m$ . Additionally, we compute the backward Euler method with  $dt = 10^{-2}$ .

The computed probability of all approaches and the corresponding absolute errors are shown in Figure 1. We use the parameter  $\sigma = 0.5$ ,  $b = 0.1$  and  $T = 1$ . The elapsed time for the PDE approach with hp-discontinuous Galerkin is 0.11 seconds, with the backward Euler method 0.30 seconds and for the Monte-Carlo approximation 162.07 seconds. The error of the Monte-Carlo approximation is the highest. Additionally, the probability is only computed at 9 points whereas with the deterministic approach at 129. There is also a significant error reduction with the hp-discontinuous Galerkin Method.

We can also calculate the first exit time density at  $x = 0$ , i.e. the time derivative of the computed probability solution. Recall that for the DG time stepping procedure we have

$$\hat{U}_m^L(x, t) = \sum_{j=0}^{r_m} \hat{U}_{m,j}^L(x) (\phi_j \circ F_m^{-1})(t)$$

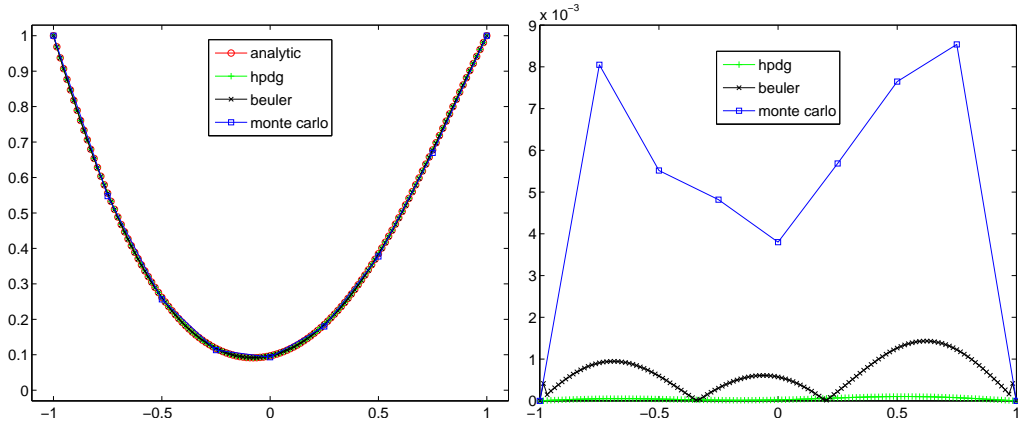


FIGURE 1. Approximation of the first exit time probability and absolute error by a scaled-Brownian motion with drift ( $\sigma = 0.5$  and  $b = 0.1$ ) from the interval  $(-1, 1)$ .

on the time interval  $I_m$ . Therefore, the time derivative is obtained by

$$\frac{\partial \hat{U}_m^L(x, t)}{\partial t} = \sum_{j=0}^{r_m} \hat{U}_{m,j}^L(x) (\phi'_j \circ F_m^{-1})(t) \frac{2}{k_m}.$$

For the backward Euler and the Monte-Carlo method we approximate the time derivative by the standard difference quotient. The first exit time density and the absolute error are plotted in Figure 2. For the deterministic approach we get smooth solution whereas the Monte-Carlo approximation oscillates. Again, the *hp*-discontinuous Galerkin time stepping yields the best results.

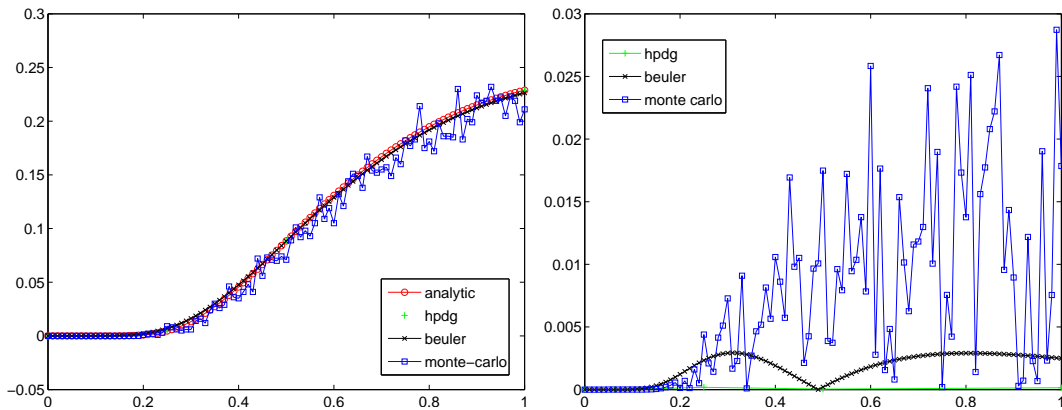


FIGURE 2. Approximation of the first exit time density and absolute error by a scaled-Brownian motion with drift ( $\sigma = 0.5$  and  $b = 0.1$ ) from the interval  $(-1, 1)$ .

The multidimensional case. In the  $n$ -dimensional case with  $n > 1$ , we consider the solution to the following system of stochastic differential equations

$$dX_t^i = b dt + \sigma dW_t^i, \quad i = 1 \dots n,$$

where the  $W^i$ 's are correlated Brownian motions with  $d\langle W^i, W^j \rangle_t = \rho dt$ ,  $i \neq j$ , with parameters  $\sigma = 0.5$ ,  $\rho = 0.5$  and  $b = 0.1$ . We consider the domain  $A = (-1, 1)^n$ . The space is discretized with  $L = 6$  levels. For the  $hp$ -discontinuous Galerkin time stepping we use again  $\log(2^{L+1})$  time steps with increasing polynomial degree  $r_m = m$ . In the Monte-Carlo method we again have  $dt = 5 \cdot 10^{-4}$ , a random sample of the size  $10^5$  and count the number of sample paths which exceed  $A$ . For  $x_0$  we choose 9 points equally spaced on a curve where all but the first dimension are fixed at  $x_i = 0$ . As a reference or ‘exact’ solution we compute the probability with the deterministic approach and  $L = 9$  levels.

In Figure 3 we plot the difference of the probability to the reference solution in 3 dimensions. The PDE approach took 30 seconds to compute, the Monte-Carlo method 360 seconds. Again the deterministic approach is more accurate and faster, although the probability is computed at about  $2 \cdot 10^6$  points.

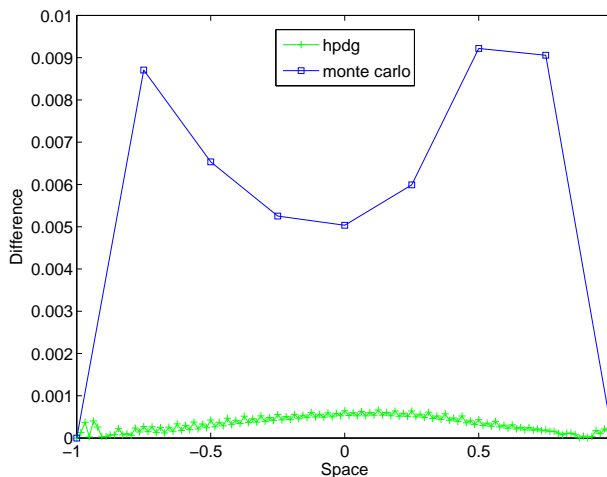


FIGURE 3. 3D absolute difference

Similar results are obtained for 5 dimensions as shown in Figure 4. Here, the elapsed time for the PDE approach is 674 seconds and the solution is computed at about  $3 \cdot 10^{10}$  points. The Monte-Carlo method needs 871 seconds.

## 5. Conclusions

First, we have shown that the first exit time probability is the unique weak solution of the backward Kolmogorov equations subject to specific initial and boundary conditions. Then, the outcomes from numerical experiments have confirmed the advantages of the presented algorithm, based on a combination of the sparse tensor product Finite Element spaces and an  $hp$ -discontinuous Galerkin method, over classical simulation techniques. Indeed, it is faster

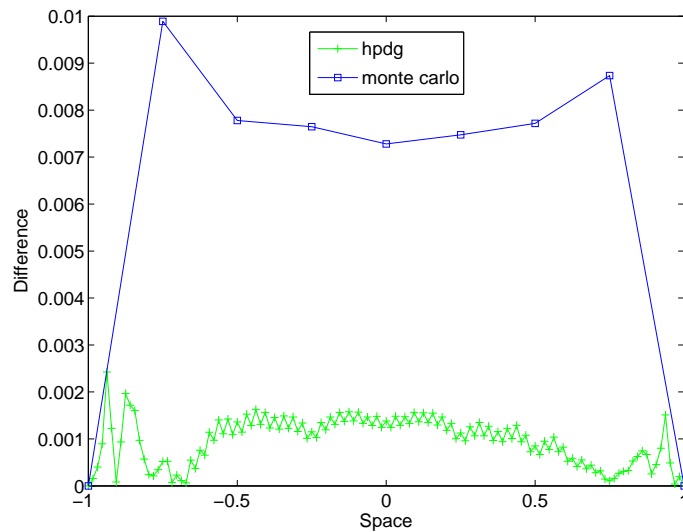


FIGURE 4. 5D Absolute Difference

and more accurate than classical Monte-Carlo methods. The  $hp$ -discontinuous Galerkin time-stepping method also improves the algorithm. Moreover, the PDE based approach has the additional advantage to provide the density and to compute the distribution of the stopping time for any starting point of the diffusion, in only one run.

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