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INITIAL-BOUNDARY VALUE PROBLEM FOR THE HEAT EQUATION—A STOCHASTIC ALGORITHM

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The initial-boundary value problem for the heat equation is solved by using an algorithm based on a random walk on heat balls. Even if it represents a sophisticated generalization of the Walk on Spheres (WOS) algorithm introduced to solve the Dirichlet problem for Laplace's equation, its implementation is rather easy. The construction of this algorithm can be considered as a natural consequence of previous works the authors completed on the hitting time approximation for Bessel processes and Brownian motion [*Ann. Appl. Probab.* **23** (2013) 2259–2289, *Math. Comput. Simulation* **135** (2017) 28–38, *Bernoulli* **23** (2017) 3744–3771]. A similar procedure was introduced previously in the paper [*Random Processes for Classical Equations of Mathematical Physics* (1989) Kluwer Academic].

The definition of the random walk is based on a particular mean value formula for the heat equation. We present here a probabilistic view of this formula.

The aim of the paper is to prove convergence results for this algorithm and to illustrate them by numerical examples. These examples permit to emphasize the efficiency and accuracy of the algorithm.

1. Introduction. In this paper, we study the Initial-Boundary Value Problem (IBVP) associated to the heat equation and the corresponding method of simulation based on the Walk on Moving Sphere Algorithm (WOMS) also called the Random Walk on Balloids. The main and historical objective is to construct an efficient approximation to the solution of the IBVP. The solution is a $\mathcal{C}^{1,2}$ function u satisfying

$$\begin{cases} \partial_t u(t,x) = \Delta_x u(t,x) & \forall (t,x) \in \mathbb{R}_+ \times \mathcal{D}, \\ u(t,x) = f(t,x) & \forall (t,x) \in \mathbb{R}_+ \times \partial\mathcal{D}, \\ u(0,x) = f_0(x) & \forall x \in \overline{\mathcal{D}}, \end{cases} \tag{1.1}$$

where f is a continuous function defined on $\mathbb{R}_+ \times \partial\mathcal{D}$, f_0 is continuous on $\mathcal{D}$ and $\mathcal{D}$ denotes a bounded finitely connected domain in $\mathbb{R}^d$. For compatibility reasons, we have also $f(0,x) = f_0(x)$.

Our work relies on the probabilistic representation for the solution of a partial differential equation. Suppose that we are looking for the solution $u(t,x)$ of some

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PDE defined on the whole space $\mathbb{R}^d$. Under a suitable hypothesis, we can use the classical form $u(t,x) = \mathbb{E}[f(t, X_t)]$ where $(X_t)_{t\in\mathbb{R}_+}$ is a stochastic process, satisfying a stochastic differential equation, and f is a known function. In order to approximate $u(t,x)$, the strong law of large numbers allows us to construct Monte Carlo methods once we are able to propose an approximating procedure for the stochastic process $(X_t)_{t\in\mathbb{R}_+}$.

The problem is more difficult when considering boundary conditions. Nevertheless, if some regularity is provided we can also find a probabilistic approach. A generic representation, for the solution of the Dirichlet problem $\mathcal{L}u(x) - k(x)u(x) = g(x)$ in a domain $\mathcal{D}$ associated to the boundary condition $u = f$ on $\partial\mathcal{D}$ (the solution does not depend on time), is

$$u(x) = \mathbb{E}\left[f(X_{\tau_\mathcal{D}}) e^{-\int_0^{\tau_\mathcal{D}} k(X_s)\,\mathrm{d}s} - \int_0^{\tau_\mathcal{D}} g(X_t) e^{-\int_0^t k(X_s)\,\mathrm{d}s}\,\mathrm{d}t \right],$$

where f, g, k are given functions, (X_t) stands for the diffusion process associated to the generator $\mathcal{L}$, $X_0 = x$ and $\tau_\mathcal{D} = \inf\{t \geq 0; X_t \in \partial\mathcal{D}\}$. We refer to several classical books for more details [1, 10, 14, 22]. The problem is hard to address as, in order to give an approximation, we need to approach the hitting time, the exit position and sometimes even the path of the process X_t up to exit the domain $\mathcal{D}$.

In particular, situations we need to characterize either the hitting time $\tau_\mathcal{D}$ or the exit position $X_{\tau_\mathcal{D}}$. The main goal of our work is to handle a more complex situation by unearthing numerical algorithms for the couple $(\tau_\mathcal{D}, X_{\tau_\mathcal{D}})$ itself.

To fix ideas and present a brief history, consider the simple Dirichlet problem for Laplace's equation in a smooth and bounded domain $\mathcal{D} \subset \mathbb{R}^d$:

$$\begin{cases} \Delta u(x) = 0 & \forall x \in \mathcal{D}, \\ u(x) = f(x) & \forall x \in \partial\mathcal{D}. \end{cases}$$

We recall the associated probabilistic representation: $u(x) = \mathbb{E}_x[f(X_{\tau_\mathcal{D}})]$ where $(X_t)_{t\geq 0}$ here stands for the d-dimensional Brownian motion starting in x. The original idea in order to approximate $u(x)$ by using the walk on spheres algorithm (WOS), was briefly introduced by Brown [3], and developed by Müller [20] and Motoo [19]; see also the textbook of Sabelfeld [24] for an interesting overview of the method. The idea consists in constructing a step by step $\mathbb{R}^d$-valued Markov chain $(x_n, n \geq 0)$ with initial point $x_0 := x$ which converges towards a limit x_∞, x_∞ and $X_{\tau_\mathcal{D}}$ being identically distributed. Let us roughly describe (x_n): first, we choose S_0 the largest sphere centered in x_0 and included in $\mathcal{D}$. The first exit point x_1 from the sphere S_0 for the Brownian motion starting from x_0 has an uniform distribution on ∂S_0 and is easy to sample.

The construction is pursued with the new starting point given by x_1 (see Figure 1). The algorithm goes on and stops while reaching the boundary $\partial\mathcal{D}$. In order to avoid an infinite sequence of hitting times, the stopping criteria of the algorithm includes a ε test: we stop the Markov chain as soon as $\delta(x_n, \partial\mathcal{D}) \leq \varepsilon$ (δ represents

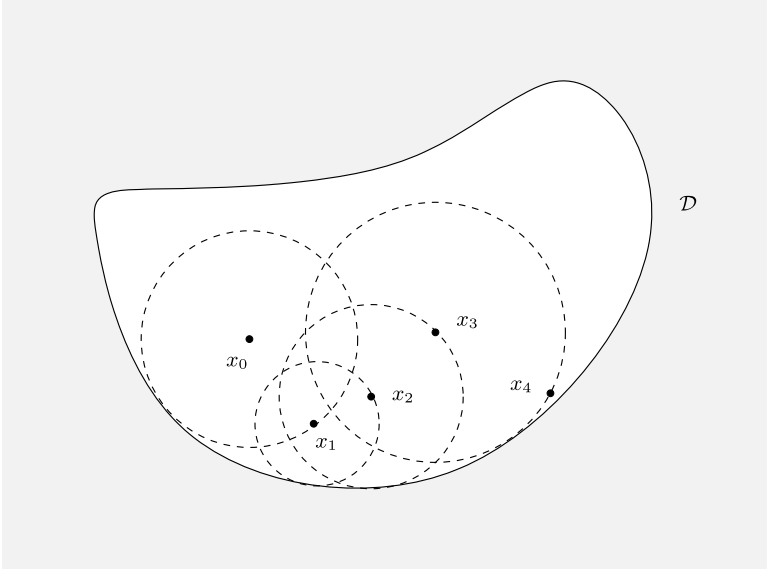

FIG. 1. *WOS algorithm.*

here the Euclidean distance in $\mathbb{R}^d$). Convergence results depending on the dimension d, on ε or/and on the regularity of $\partial\mathcal{D}$ can be found in Müller [20], Motoo [19], Sabelfeld [24] and Mascagni and Hwuang [17]. Generalization of this result to a constant drift, by means of convergence theorems for discrete-time martingales, was proposed in the work of Villa-Morales [28, 29]. Binder and Braverman [2] gave also the complete characterization of the rate of convergence for the WOS in terms of the local geometry of $\mathcal{D}$. Other elliptic problems have been studied by Gurov, Whitlock and Dimov [12].

If needed, we can also approach the boundary hitting time by using the explicit form of its probability distribution function. However, a real difficult leap appears when we want to move from the simulation of X_t to the simulation of (t, X_t). For example, if the domain is a sphere then $X_{\tau_\mathcal{D}}$ can be simulated by the uniform random variable on the $\partial\mathcal{D}$ while $\tau_\mathcal{D}$ has an explicit p.d.f. function which is not well suited for numerical approaches as it depends on the Bessel function. Nevertheless, acceptance/rejection sampling methods can be used in order to simulate $\tau_\mathcal{D}$.

In previous works [4–6], the authors discussed the connection between the hitting times of the Bessel process and Brownian ones and introduced a new technique for approximating both the hitting time and the exit position. These previous studies on the hitting time form the foundation of our current work. We take inspiration from these results by proposing an adapted algorithm. It involves a random walk on heat balls belonging to the domain $[0, t] \times \mathcal{D}$ (see (1.2) or [8], page 53, for a definition of the heat ball) which approaches (τ_D, X_{τ_D}) in general domains.

Thus we obtain a method for approximating the solution of the equation (1.1). The description of the approximation error term and a sharp estimation of the rate of convergence become then essential challenges. The aim of our work is to consider these questions in a quite general framework (both for the space dimension and the geometry of the domain). Various Monte Carlo methods have already been introduced in order to approximate the solution of a nonstationary heat equation. A first family of methods concerns random walks inside the domain: Haji-Sheikh and Sparrow [13] proposed a floating walk using Euclidean spheres and their corresponding exit times. In order to simplify the expression of these hitting times, the spheres can be replaced by heat balls also called balloids. Such an algorithm has been presented in details in Ermakov, Nekrutkin and Sipin [7] and is similar to the random walk which holds our attention here.

Let us also mention at this stage that a second family of random walks $(\tau_n, Y_n)_{n\geq 0}$ can be used for solving the initial-boundary value problem in the heat equation context: the random walk on the boundary $[0,t]\times\partial\mathcal{D}$. A nicely written description of the method can be found in [26].

Let us now introduce the main results concerning the algorithm random walk on heat balls which approximates $(\tau_{\mathcal{D}}, X_{\tau_{\mathcal{D}}})$, X being a d-dimensional Brownian motion. We first introduce some preliminary notation: we recall that $\delta(x,\partial\mathcal{D})$ is the Euclidean distance between the point x and the boundary of the domain and introduce the function $\alpha(u,v)=\min(u,\frac{e}{2d}\delta^2(v,\partial\mathcal{D}))$. In the following, $(U_n)_{n\geq 1}$ stands for a sequence of independent uniformly distributed random vectors on $[0,1]^{\lfloor d/2\rfloor+1}$, Π_n^U denote the product of all its coordinates, $(G_n)_{n\geq 1}$ is a sequence of independent standard Gaussian r.v. and $(V_n)_{n\geq 1}$ is a sequence of independent uniformly distributed random vectors on the unit sphere of dimension d, centered on the origin. We assume these three sequences to be independent. Let us define:

$$R_{n+1} := (\Pi_{n+1}^U)^{2/d}\exp\left\{-\left(1-\frac{2}{d}\left\lfloor\frac{d}{2}\right\rfloor\right)G_{n+1}^2\right\}$$

and construct a sequence $(T_n, X_n)_{n\geq 0}$ by the following procedure (Figure 2).

ALGORITHM

Initialisation: Fix $\varepsilon>0$. The initial value of the sequence (T_n,X_n) is $(T_0,X_0)=(t,x)$.

Step n: The sequence is defined by recurrence as follows: for $n\geq 0$,

$$\begin{cases} T_{n+1}=T_n-\alpha(T_n,X_n)R_{n+1},\\ X_{n+1}=X_n+2\sqrt{\alpha(T_n,X_n)}\psi_d(R_{n+1})V_{n+1},\end{cases}$$

where $\psi_d(t)=\sqrt{t\log(t^{-d/2})}$.

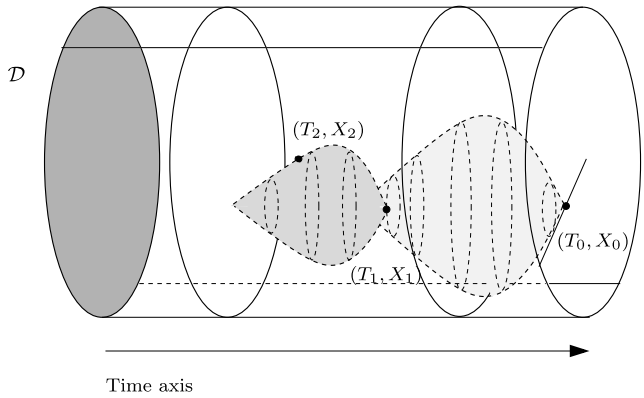

FIG. 2. *Markov chain* $(T_n, X_n)_{n\geq 0}$.

Stop. If $\alpha(T_n, X_n) \leq \varepsilon$ then $\mathcal{N}_\varepsilon = n$:
1. If $\delta^2(X_{\mathcal{N}_\varepsilon}, \partial\mathcal{D}) \leq \frac{2\varepsilon d}{e}$ then choose $X_\varepsilon \in \partial\mathcal{D}$ such that

$$\delta(X_{\mathcal{N}_\varepsilon}, X_\varepsilon) = \delta(X_{\mathcal{N}_\varepsilon}, \partial\mathcal{D})$$

and define $T_\varepsilon := T_{\mathcal{N}_\varepsilon}$.
2. If $\delta^2(X_{\mathcal{N}_\varepsilon}, \partial\mathcal{D}) > \frac{2\varepsilon d}{e}$ then set $T_\varepsilon = 0$ and $X_\varepsilon := X_{\mathcal{N}_\varepsilon}$.

Algorithm outcomes: We get thus $(T_\varepsilon, X_\varepsilon)$ and $\mathcal{N}_\varepsilon$ the number of steps.

This algorithm is quite similar to the random walk on moving spheres but in order to solve the IBVP instead of the Dirichlet problem, the spheres are replaced by spheroïds (heat balls). The spheroïd centered in $(t, x) \in \mathbb{R}_+ \times \mathbb{R}^d$ with parameter $a > 0$ is defined by

$$\mathcal{S}_a(t, x) = \big\{(s, y) \in [t - a, t] \times \mathbb{R}^d : \delta(x, y) = 2\sqrt{a}\psi_d(s/a)\big\}. \tag{1.2}$$

See Figure 2 for an illustration. Let us notice that the set $\mathcal{S}_a(t, x)$ converges towards the point (t, x) as the parameter a tends to 0. We now present the random walk: in order to evaluate $u(t, x)$, solution to (1.1), we choose the value (t, x) as initial value of the $[0, t] \times \mathcal{D}$-valued random walk (T_n, X_n). At each step, we consider the exit time and exit position from the spheroïd $\mathcal{S}_a(T_n, X_n)$ for the time-reverting Brownian motion starting at time T_n in X_n. The exit problem permits to obtain (T_{n+1}, X_{n+1}) with $T_{n+1} \leq T_n$. Let us note that the parameter a (depending on n) is chosen as large as possible under the constraint: $\mathcal{S}_a(T_n, X_n) \subset [0, t] \times \mathcal{D}$. Such a parameter is represented by the function α appearing in the algorithm. Finally, the procedure is stopped as soon as the Markov chain reaches an ε-neighborhood of the boundary and the outcome then corresponds to its *projection* on the boundary, denoted by $(T_\varepsilon, X_\varepsilon)$.

We propose an approximation of the solution to (1.1) by using the definition:

$$u^\varepsilon(t, x) = \mathbb{E}_{(t,x)}\big[f(T_\varepsilon, X_\varepsilon)1_{\{X_\varepsilon \in \partial\mathcal{D}\}}\big] + \mathbb{E}_{(t,x)}\big[f_0(X_\varepsilon)1_{\{X_\varepsilon \notin \partial\mathcal{D}\}}\big]$$

for $(t,x) \in [0,T] \times \overline{\mathcal{D}}$. We will prove the convergence of this approximation in Proposition 4.1.

CONVERGENCE RESULT. *Let us assume that the initial-boundary value problem (1.1) admits an unique $\mathcal{C}^{1,2}([0,T] \times \mathcal{D})$-solution u, defined by (3.3). We introduce the approximation u^ε given by (4.2). Then u^ε converges towards u, as $\varepsilon \to 0$, uniformly with respect to (t,x). Moreover, there exist $\kappa_{T,\mathcal{D}}(u) > 0$ and $\varepsilon_0 > 0$ such that*

$$\left|u(t,x) - u^\varepsilon(t,x)\right| \le \kappa_{T,\mathcal{D}}(u)\sqrt{\varepsilon} \qquad \forall \varepsilon \le \varepsilon_0, (t,x) \in [0,T] \times \mathcal{D}.$$

The main result, based on the construction of a submartingale related to the Riesz potential, describes the convergence rate of the algorithm.

EFFICIENCY RESULT. *Let $\mathcal{D} \subset B(0,1)$ be a 0-thick domain. The number of steps $\mathcal{N}_\varepsilon$, of the approximation algorithm, is almost surely finite. Moreover, there exist constants $C > 0$ and $\varepsilon_0 > 0$ both independent of (t,x) such that*

$$\mathbb{E}[\mathcal{N}_\varepsilon] \le C|\log \varepsilon| \qquad \text{for all } \varepsilon \le \varepsilon_0.$$

The material is organized as follows. In the second section, we present some well-known mean value properties for the heat equation, which play a central role in the definition of the algorithm and emphasize arguments of proof directly related to this particular algorithmic and probabilistic approach. The third section constructs the random walk on heat balls used to solve the initial-boundary value problem. In Section 4, we introduce the stopping procedure of the algorithm and prove the convergence result. The rate of the algorithm is analyzed. We end up the paper with numerical results for two particular domains. These illustrations corroborate the accuracy of the algorithm.

2. A spherical mean value property associated to the heat equation. In this section, we will discuss the link between solutions of the heat equation and a particular version of the mean value property. This link is also an essential tool in the study of the classical Dirichlet problem.

Let us first note that due to the time reversion, the solution of the initial-boundary value problem for the heat equation is directly related to the solution of the terminal-boundary value problem for the backward heat equation (heat equation with negative diffusion). Due to this essential property, we are going to first present a mean value property for the *backward heat equation* and then deduce a similar property for the heat equation.

Let A be an open nonempty set of $\mathbb{R}_+ \times \mathbb{R}^d$.

DEFINITION 2.1. A function $h : A \mapsto \mathbb{R}$ is said to be a *co-temperature* in A if h is a $\mathcal{C}^{1,2}$-function satisfying

$$\partial_t h(t,x) + \Delta_x h(t,x) = 0 \qquad \forall (t,x) \in A. \tag{2.1}$$

PROPOSITION 2.2. *Let $A \subset \mathbb{R}_+ \times \mathbb{R}^d$ be a nonempty open set. If a function h is a* co-temperature *in A, then it has the following mean value property*:

$$h(t,x) = \frac{1}{2\pi^{d/2}} \iint_{(s,y)\in\,]0,1[\times\mathbb{S}^d} \frac{1}{s} h\big(t+\alpha s, x + 2\sqrt{\alpha}\psi_d(s)y\big)\psi_d^d(s)\,\mathrm{d}\sigma(y)\,\mathrm{d}s, \tag{2.2}$$

where $\mathbb{S}^d$ is the d-dimensional sphere of radius 1, σ is the Lebesgue measure on $\mathbb{S}^d$ and

$$\psi_d(t) = \sqrt{t\log\big(t^{-d/2}\big)}, \qquad t \in\,]0,1[. \tag{2.3}$$

Equation (2.2) is satisfied for any $\alpha > 0$ such that

$$[t, t+\alpha] \times \overline{B\big(x, 2\sqrt{\alpha d/(2e)}\big)} \subset A.$$

Here, $\overline{B(x,r)}$ stands for the Euclidean ball centered in x of radius r, that is, $\overline{B(x,r)} = \{x \in \mathbb{R}^d \text{ s.t. } \|x\| \le r\}$.

Let us just explain this mean value property: the value of the temperature $h(t,x)$ is directly related to the mean of the temperature $h(s,y)$ where (s,y) belongs to the boundary of the heat ball (spheroïd) centered in (t,x) and whose size is parametrized by α. That is why the expression (2.2) is valid for any α which insures that the ball is contained in the domain A.

The Gauss mean value theorem and its converse due to Koebe permit to characterize the Laplace equation. Pini [16, 23] introduced an analogue of Gauss' formula in the one-dimensional heat equation context and Montaldo [18] extended the study to higher dimensions. Fulks [11] proved the same result apparently without knowledge of the results of Pini. These authors pointed out the following fundamental mean value over heat spheres for temperatures:

$$h(t,x) = \frac{1}{(4\pi\alpha)^{d/2}} \int_{\mathcal{S}_\alpha(t,x)} Q(x-y, t-s)h(s,y)\,\mathrm{d}\sigma_{\mathcal{S}}, \tag{2.4}$$

where the spheroïd $\mathcal{S}_\alpha(t,x)$ is defined by (1.2), $\sigma_{\mathcal{S}}$ stands for its surface area measure and Q is given by

$$Q(y,s) = \|y\|^2\sqrt{4\|y\|^2s^2 + \big(\|y\|^2 - 2ds^2\big)^2} \qquad \text{for } (s,y) \in \mathbb{R}_+ \times \mathbb{R}^d.$$

Similar results were also proven by Smyrnélis [27] and Kuptsov [15]. We suggest the reading of the interesting historical overview written by Netuka and Vesely [21] and the presentation of the link between temperatures and heat balls in the textbook of Watson [30]. The explicit expression of the mean value formula for the co-temperature pointed out in Proposition 2.2 seems quite different from the famous expression (2.4). In fact, time reversion and tedious computations (change of variables) permit to prove that both expressions are equivalent.

Let us also notice that the mean value formula (2.2) is different and more general than the classical formula associated to the heat equation in balloïds (see, for

instance, Theorem 3 on page 53 in [8]). Nevertheless, after some transformations on (2.2), it is possible to obtain the classical mean value property. These transformations consist in time reversion and integration of the *radius* of spheroïd with respect to a particular probability distribution function with compact support.

The statement of Proposition 2.2 is classical in analysis; nevertheless, we opt for a quite different presentation emphasizing the link between the mean value property and exit problems for stochastic processes.

PROOF OF PROPOSITION 2.2. Let $a \in \mathbb{R}_+$ be defined by $a = \alpha^{d/2}\Gamma(d/2) \times 2^{d/2-1}$ and let us consider the associated function

$$\psi_{a,d}(t) := \sqrt{2t \log\Big(\frac{a}{\Gamma(d/2)t^{d/2}2^{d/2-1}}\Big)}.$$

We introduce $(W_t, t \geq 0)$ a standard d-dimensional Brownian motion and define by $\tau_{a,d}$ the following hitting time:

$$\tau_{a,d} = \inf\big\{t \geq 0 : \|W_t\| = \psi_{a,d}(t)\big\}.$$

Let us just notice that this hitting time is bounded by $\alpha = (\frac{a}{\Gamma(d/2)2^{d/2-1}})^{2/d}$ and its distribution function is given by Proposition 5.1 in [5]

$$p_{a,d}(t) = \frac{1}{2at}\psi_{a,d}^d(t), \qquad 0 \leq t \leq \alpha. \tag{2.5}$$

Furthermore, the exit location $W_{\tau_{a,d}}$ is uniformly distributed on the sphere of radius $\psi_{a,d}(\tau_{a,d})$. Let us consider h a co-temperature on A. By Itô's formula, we obtain

$$\begin{aligned} h(t+\tau_{a,d}, x+\sqrt{2}W_{\tau_{a,d}}) = h(t,x) &+ \int_0^{\tau_{a,d}} \partial_t h(t+s, x+\sqrt{2}W_s)\,\mathrm{d}s \\ &+ \sqrt{2}\int_0^{\tau_{a,d}} \partial_x h(t+s, x+\sqrt{2}W_s)\,\mathrm{d}W_s \\ &+ \int_0^{\tau_{a,d}} \Delta_x h(t+s, x+\sqrt{2}W_s)\,\mathrm{d}s. \end{aligned}$$

If a is small enough, then there exists a compact set K such that $(t,x)+K \subsetneq A$ and $\{(s,y) \in \mathbb{R}_+ \times \mathbb{R}^d : \|y\| \leq \psi_{a,d}(s), 0 \leq s \leq \alpha\} \subset K$. Let us note τ_K the first exit time of the domain K for the process (s, W_s). Using the fact that h is a co-temperature in A, in particular, the continuity of $\partial_x h$ is known, we can prove that the stochastic integral introduced in the Itô formula $r \mapsto \int_0^{r\wedge\tau_K} \partial_x h(t+s, x+\sqrt{2}W_s)\,\mathrm{d}W_s$ is a martingale. Hence combining the stopping time theorem and the a.s. property $\tau_{a,d} \leq \tau_K < \infty$, we obtain

$$h(t,x) = \mathbb{E}\big[h(t+\tau_{a,d}, x+\sqrt{2}W_{\tau_{a,d}})\big].$$

By (2.5), we get

$$h(t,x) = \frac{1}{\sigma(\mathbb{S}^d)}\int_0^\alpha \int_{\mathbb{S}^d} h\big(t+u, x+\sqrt{2}\psi_{a,d}(u)y\big)\frac{1}{2au}\psi_{a,d}^d(u)\,\mathrm{d}\sigma(y)\,\mathrm{d}u.$$

We introduce the change of variable $u = \alpha s$, such that $s \in]0, 1[$, and observe that $\psi_{a,d}(\alpha s) = \sqrt{2\alpha}\psi_d(s)$ where ψ_d is defined by (2.3). We get

$$h(t,x) = \frac{1}{\sigma(\mathbb{S}^d)} \int_0^1 \int_{\mathbb{S}^d} h\big(t+\alpha s, x+\sqrt{2}\psi_{a,d}(\alpha s)y\big) \frac{1}{2as} \psi_{a,d}^d(\alpha s)\, \mathrm{d}\sigma(y)\, \mathrm{d}s$$
$$= \frac{1}{\sigma(\mathbb{S}^d)} \int_0^1 \int_{\mathbb{S}^d} h\big(t+\alpha s, x+2\sqrt{\alpha}\psi_d(s)y\big) \frac{2^{d/2}\alpha^{d/2}}{2as} \psi_d^d(s)\, \mathrm{d}\sigma(y)\, \mathrm{d}s.$$

Using both the explicit expression of $\alpha^{d/2}$ and the classical formula $\sigma(\mathbb{S}^d) = 2\pi^{d/2}/\Gamma(d/2)$ leads to (2.2). □

The reverse statement of the preceding result can also be proved. The first step consists of the following.

PROPOSITION 2.3. *If h satisfies the mean value property (2.2) and is a $\mathcal{C}^{1,2}$-function for any $(t,x) \in A$ and $\alpha > 0$ such that*

$$[t, t+\alpha] \times \overline{B\big(x, 2\sqrt{\alpha d/(2e)}\big)} \subset A,$$

then h is a cotemperature *in A.*

In the statement of Proposition 2.3, which corresponds to an analogue of the Koebe result for Laplace's equation, the function h is assumed to be smooth. Such result can be generalized to mean value properties associated to other parabolic equations provided that h satisfies suitable regularity conditions (see, for instance, Sabelfeld and Shalimova [25], Section 2.4). In fact, the reverse statement can be highly improved for the heat equation. In the pioneer work of Fulks [11], the author points out that continuous functions h (in the intended domain) satisfying the mean value property on spheroïds, satisfy the parabolic maximum principle. It is therefore easy to conclude that h is a $\mathcal{C}^{1,2}$-function. We consider relevant to present here a simple proof of Proposition 2.3 related to the particular choice of the mean value expression (2.2) and to its associated probabilistic interpretation.

PROOF OF PROPOSITION 2.3. Let us consider the function $H : [0, \sqrt{\alpha}] \to \mathbb{R}$ defined by

$$H(r) = h\big(t + r^2 s, x + 2r\psi_d(s)y\big)$$

for any $(s, y) \in [0,1] \times \mathbb{S}^d$. Using the Taylor expansion, we get

$$H(\sqrt{\alpha}) = H(0) + H'(0)\sqrt{\alpha} + \frac{\alpha}{2}H''(0) + o(\alpha), \tag{2.6}$$

where $o(\alpha)$ is uniform with respect to both s and y variables. The derivatives of H can be computed explicitly and we get

$$H(0) = h(t,x), \qquad H'(0) = 2\psi_d(s) \sum_{j=1}^{d} \partial_{x_j} h(t,x) y_j,$$

$$H''(0) = 2s\partial_t h(t,x) + 4\psi_d^2(s) \sum_{1\le i,j\le d} \partial^2_{x_i x_j} h(t,x) y_i y_j.$$

Applying the mean value property to both sides of (2.6), we obtain

$$\sum_{j=1}^{d} \partial_{x_j} h(t,x) A_j^0 + \partial_t h(t,x) A_1 + \sum_{1\le i,j\le d} \partial_{x_i x_j} h(t,x) A_{i,j} = o(\alpha), \tag{2.7}$$

where

$$A_j^0 = \frac{2\sqrt{\alpha}}{2\pi^{d/2}} \iint_{(s,y)\in[0,1]\times\mathbb{S}^d} \frac{1}{s} \psi_d^{d+1}(s) y_j \, \mathrm{d}\sigma(y)\, \mathrm{d}s,$$

$$A_1 = \frac{\alpha}{2\pi^{d/2}} \iint_{(s,y)\in[0,1]\times\mathbb{S}^d} \psi_d^{d}(s) \, \mathrm{d}\sigma(y)\, \mathrm{d}s,$$

$$A_{i,j} = \frac{\alpha}{\pi^{d/2}} \iint_{(s,y)\in[0,1]\times\mathbb{S}^d} \frac{1}{s} \psi_d^{d+2}(s) y_i y_j \, \mathrm{d}\sigma(y)\, \mathrm{d}s.$$

By symmetry arguments, we have $A_j^0 = 0$ and $A_{i,j} = 0$ for $i \neq j$. Let X_d be a random variable whose probability distribution function is

$$p_d(t) = \frac{1}{\Gamma(d/2)t} \psi_d^d(t) 1_{[0,1]}(t).$$

Let us just notice that $p_d(t) = \alpha p_{a,d}(\alpha t)$, $p_{a,d}$ being defined by (2.5). Then $X_d = e^{-G}$ where G is a random variable which has the gamma distribution of parameters $(d+2)/2$ and $2/d$. In particular, X_d has the same distribution as $(U_1 \cdots U_{(d+2)/2})^{2/d}$ if d is even [here $(U_i)_{i\in\mathbb{N}}$ is a sequence of standard uniform independent random variables] and X_d has the same distribution as $(U_1 \cdots U_{\lfloor d+2 \rfloor/2})^{2/d} e^{-N^2/d}$ if d is odd [here N is a standard Gaussian r.v. independent of the sequence $(U_i)_i$]. Therefore, if d is even, we deduce

$$A_1 = \frac{\alpha\Gamma(d/2)}{2\pi^{d/2}} \sigma(\mathbb{S}_1) \mathbb{E}[X_d] = \alpha \mathbb{E}[X_d] = \alpha \mathbb{E}\big[U_1^{2/d}\big] \mathbb{E}\big[U_2^{2/d}\big] \cdots \mathbb{E}\big[U_{(d+2)/2}^{2/d}\big]$$

$$= \alpha \left(\frac{d}{d+2}\right)^{(d+2)/d}.$$

For the odd case,

$$A_1 = \alpha \mathbb{E}[X_d] = \alpha \mathbb{E}\big[U_1^{2/d}\big] \mathbb{E}\big[U_2^{2/d}\big] \cdots \mathbb{E}\big[U_{\lfloor d+2 \rfloor/2}^{2/d}\big] \mathbb{E}\big[e^{-N^2/d}\big]$$

$$= \alpha \left(\frac{d}{d+2}\right)^{\lfloor d+2 \rfloor/d} \mathbb{E}\big[e^{-N^2/d}\big].$$

Let us now compute $A_{i,i}$ for $1 \le i \le n$. First, we observe that

$$\int_{\mathbb{S}^d} y_i^2 \, \mathrm{d}\sigma(y) = \frac{1}{d} \sum_{j=1}^{d} \int_{\mathbb{S}^d} y_j^2 \, \mathrm{d}\sigma(y) = \frac{\sigma(\mathbb{S}^d)}{d} = \frac{2\pi^{d/2}}{d\Gamma(d/2)}.$$

So using a convenient change of variable, we get

$$\begin{aligned} A_{i,i} &= \frac{\alpha}{\pi^{d/2}} \frac{2\pi^{d/2}}{d\Gamma(d/2)} \int_0^1 \frac{1}{s} \psi_d^{d+2}(s) \, \mathrm{d}s \\ &= \frac{2\alpha(d+2)}{d^2\Gamma(d/2)} \Gamma\big((d+2)/2\big) \int_0^1 \frac{1}{\Gamma((d+2)/2)} t^{(d+2)/d} \frac{1}{t} \psi_{d+2}^{d+2}(t) \, \mathrm{d}t \\ &= \alpha \frac{d+2}{d} \mathbb{E}\big[X_{d+2}^{(d+2)/d}\big] = \alpha \left(\frac{d}{d+2} \right)^{(d+2)/d} \qquad \text{if } d \text{ is even,} \end{aligned}$$

and $A_{i,i} = \alpha(\frac{d}{d+2})^{\lfloor d+2 \rfloor/d} \mathbb{E}[e^{-N^2/d}]$ if d is odd. So we note that for any $d \in \mathbb{N}^*$, we proved that

$$A_j^0 = 0, \qquad A_{i,j} = \delta_{ij} A_1,$$

where δ_{ij} is the Kronecker's symbol. Equation (2.7) leads therefore to (2.1). □

All results presented so far in this section have an important advantage, they can be adapted to other situations for instance by looking backward in time, or equivalently time reverting. This observation permits to study properties of the heat equation.

DEFINITION 2.4. A function $h : A \mapsto \mathbb{R}$ is said to be a *temperature* in A if h is a $\mathcal{C}^{1,2}$-function satisfying the heat equation:

$$\partial_t h(t,x) - \Delta_x h(t,x) = 0 \qquad \forall (t,x) \in A. \tag{2.8}$$

By Proposition 2.2 and Proposition 2.3, we obtain the following.

THEOREM 2.5. 1. *Let $A \subset \mathbb{R}_+ \times \mathbb{R}^d$ be a nonempty open set. If a function h is a* temperature *in A, then it has the following mean value property*:

$$h(t,x) = \frac{1}{2\pi^{d/2}} \iint_{(s,y) \in]0,1[\times \mathbb{S}^d} h\big(t - \alpha s, x + 2\sqrt{\alpha} \psi_d(s) y\big) \frac{\psi_d^d(s)}{s} \, \mathrm{d}\sigma(y) \, \mathrm{d}s, \tag{2.9}$$

where $\mathbb{S}^d$ is the d-dimensional sphere of radius 1, σ is the Lebesgue measure on $\mathbb{S}^d$ and ψ_d is defined in (2.3). Equation (2.9) is satisfied for any $\alpha > 0$ such that $[t-\alpha, t] \times \overline{B(x, 2\sqrt{\alpha d/(2e)})} \subset A$.

2. *If h satisfies the mean value property (2.9) and is a $\mathcal{C}^{1,2}$-function for any $(t,x) \in A$ and $\alpha > 0$ such that $[t-\alpha, t] \times \overline{B(x, 2\sqrt{\alpha d/(2e)})} \subset A$ then h is a* temperature *in A.*

3. Solving the initial-boundary value problem. This section deals with existence and uniqueness for solutions of the initial-boundary value problem (1.1) in a bounded domain $\mathcal{D}$. These results are deeply related to the existence of a particular time-discrete martingale: we define $M_n := (T_n, X_n)$ a sequence of $\mathbb{R}_+ \times \mathcal{D}$-valued random variables. A similar martingale was previously described in the textbook of Ermakov, Nekruktin and Sipin [7]: we just present or recall here relevant properties and classical results associated to this random process in order to present a comprehensive study of the random walk on moving sphere algorithm. In order to define this sequence, we introduce $\delta(x, \partial\mathcal{D})$, the Euclidean distance between the point x and the boundary of the domain. We also introduce the function α given by

$$\alpha(u, v) = \min\left(u, \frac{e}{2d}\delta^2(v, \partial\mathcal{D})\right). \tag{3.1}$$

Let us consider:

- $(U_n)_{n\geq 1}$ a sequence of independent uniformly distributed random vectors on $[0, 1]^{\lfloor d/2\rfloor+1}$. We denote by Π_n^U the product of all coordinates of U_n.
- $(G_n)_{n\geq 1}$ a sequence of independent standard Gaussian r.v.
- $(V_n)_{n\geq 1}$ a sequence of independent uniformly distributed random vectors on the unit sphere of dimension d, centered at the origin.

Further, we assume that these three sequences are independent. We define by $\mathcal{F}_n$ the natural filtration generated by the sequences (U_n), (G_n) and (V_n). Let $\mathcal{F}_0$ note the trivial σ-algebra. Let us introduce

$$R_{n+1} := \left(\Pi_{n+1}^U\right)^{2/d} \exp\left\{-\left(1 - \frac{2}{d}\left\lfloor \frac{d}{2}\right\rfloor\right)G_{n+1}^2\right\}.$$

The initial value of the sequence (T_n, X_n) is then $(T_0, X_0) = (t, x)$ and the sequence is defined by recurrence as follows: for $n \geq 0$,

$$\begin{cases} T_{n+1} = T_n - \alpha(T_n, X_n)R_{n+1}, \\ X_{n+1} = X_n + 2\sqrt{\alpha(T_n, X_n)}\psi_d(R_{n+1})V_{n+1}. \end{cases} \tag{3.2}$$

Let us first note that, due to the definition, the sequence (T_n, X_n) belongs always to the closed set $[0, t] \times \overline{\mathcal{D}}$: the sequence is therefore bounded. Moreover, as soon as M_n reaches the boundary of $[0, t] \times \overline{\mathcal{D}}$ its value is frozen.

LEMMA 3.1. *If h belongs to $\mathcal{C}^{1,2}([0, t] \times \overline{\mathcal{D}})$ and if it is a temperature in $[0, t] \times \mathcal{D}$, then $\mathcal{M}_n := h(T_n, X_n)$ is a bounded $\mathcal{F}$-martingale.*

PROOF. Since h is a continuous function on a compact set, it is bounded. Therefore, the stochastic process $\mathcal{M}_n$ itself is bounded. We obtain

$$\mathbb{E}[\mathcal{M}_{n+1}|\mathcal{F}_n] = \mathbb{E}\big[h(T_{n+1}, X_{n+1})|\mathcal{F}_n\big] =: H(T_n, X_n),$$

where

$$H(u,v)=\mathbb{E}\big[h\big(u-\alpha(u,v)R_{n+1},v+2\sqrt{\alpha(u,v)}\psi_d(R_{n+1})V_{n+1}\big)\big].$$

Since the p.d.f. of R_{n+1} is given by $f_R(s)=\frac{1}{\Gamma(d/2)}\frac{\psi_d^d(s)}{s}1_{[0,1]}(s)$ and since V_{n+1} is uniformly distributed on the sphere, we obtain

$$H(u,v)=\frac{1}{\Gamma(d/2)\sigma(\mathbb{S}^d)}\times\iint_{(s,y)\in]0,1[\times\mathbb{S}^d}h\big(t-\alpha(u,v)s,x+2\sqrt{\alpha(u,v)}\psi_d(s)y\big)\frac{\psi_d^d(s)}{s}\,\mathrm{d}\sigma(y)\,\mathrm{d}s.$$

If h belongs to $\mathcal{C}^{1,2}([0,t]\times\overline{\mathcal{D}})$ and if it is a temperature in $[0,t]\times\mathcal{D}$, then Theorem 2.5 implies the mean value property. Hence $H(u,v)=h(u,v)$. We deduce easily that

$$\mathbb{E}[\mathcal{M}_{n+1}|\mathcal{F}_n]=h(T_n,X_n)=\mathcal{M}_n\qquad\text{a.s.}\qquad\square$$

LEMMA 3.2. *The process $M_n=(T_n,X_n)$ converges almost surely as $n\to\infty$ to a limit (T_∞,X_∞) that belongs to the set $\{0\}\times\overline{\mathcal{D}}\cup]0,t[\times\partial\mathcal{D}$.*

PROOF. Let us consider the function $h(t,x)=x_i$ the ith coordinate of $x\in\mathbb{R}^d$. We observe that h is a temperature and belongs to $\mathcal{C}^{1,2}(\mathbb{R}_+,\mathbb{R}^d)$. By Lemma 3.1, we deduce that $\mathcal{M}_n:=h(T_n,X_n)=X_n(i)$, the ith coordinate of X_n, is a bounded martingale therefore it converges a.s. towards $X_\infty(i)$. Since all coordinates converge, we deduce that $X_n\to X_\infty$ a.s.

Moreover, since T_n is a nonincreasing sequence of nonnegative random times, it converges a.s. towards a r.v. T_∞ which belongs to $[0,t]$. The sequence (T_n,X_n) belongs to the closed set $[0,t]\times\overline{\mathcal{D}}$, consequently its limit belongs to the same set.

Since the function α is continuous, we obtain that $\alpha_n:=\alpha(T_n,X_n)$ converge a.s. to α_∞.

Let us assume that there exist $\eta_1>0$ and $\eta_2>0$ such that $\mathbb{P}(\alpha_\infty>\eta_1)>\eta_2$. The a.s. convergence implies the convergence in probability; consequently, there exists $n_0\in\mathbb{N}$ such that $\mathbb{P}(\alpha_n>\eta_1/2)>\eta_2/2$ for any $n\geq n_0$. Moreover, the definition of the random walk algorithm (3.2) implies the existence of a parameter $0<\gamma<1$ such that $\mathbb{P}(\|X_{n+1}-X_n\|>\gamma\alpha_n)>1-\eta_2/4$ for any $n\geq 0$. Combining these two properties, we obtain that

$$\mathbb{P}\big(\|X_{n+1}-X_n\|>\gamma\eta_1/2\big)>\eta_2/4$$

for any $n\geq n_0$ which contradicts the almost sure convergence of (X_n). We deduce that $\alpha_\infty=0$ a.s. and, therefore, $(T_\infty,X_\infty)\in\{0\}\times\overline{\mathcal{D}}\cup]0,t[\times\partial\mathcal{D}$. $\square$

PROPOSITION 3.3 (Uniqueness). *Set $T>0$. Let u be a $\mathcal{C}^{1,2}([0,T]\times\mathcal{D})$-function satisfying the initial-boundary value problem (1.1) and continuous with*

respect to both variables on $[0,T]\times\overline{\mathcal{D}}$. *Then* u *is unique and given by the following expression*: *for* $(t,x)\in[0,T]\times\overline{\mathcal{D}}$,

$$u(t,x)=\mathbb{E}_{(t,x)}\big[f(T_\infty,X_\infty)1_{\{X_\infty\in\partial\mathcal{D}\}}\big]+\mathbb{E}_{(t,x)}\big[f_0(X_\infty)1_{\{X_\infty\notin\partial\mathcal{D}\}}\big]. \tag{3.3}$$

PROOF. By Lemma 3.1, the process $\mathcal{M}_n$ is a bounded martingale. Moreover, Lemma 3.2 implies that (T_n,X_n) converges to (T_∞,X_∞). Since u is a continuous function, we deduce that $\mathcal{M}_n$ converges a.s. and in L^2 towards $u(T_\infty,X_\infty)$. In particular, the martingale property leads to

$$u(t,x)=\mathbb{E}\big[u(T_\infty,X_\infty)\big].$$

In order to conclude it suffices to use the initial and boundary conditions. Indeed Lemma 3.2 ensures that (T_∞,X_∞) belongs to the set $\{0\}\times\overline{\mathcal{D}}\cup]0,t[\times\partial\mathcal{D}$. □

We refer to Friedman [9] for the existence of a solution to the initial-boundary value problem (1.1). More precisely, if the following particular conditions are fulfilled:

- f and f_0 are continuous functions such that $f(0,x)=f_0(x)$,
- the domain has an outside strong sphere property,

then there exists a smooth solution u to (1.1): $u\in\mathcal{C}^\infty(\mathbb{R}_+\times\mathcal{D},\mathbb{R})$. This statement results from a combination of Theorem 9 on page 69 and Corollary 2 on page 74 in [9].

4. Approximation of the solution for an initial-boundary value problem. The aim of this section is to construct an algorithm which approximates $u(t,x)$, the solution of an initial-boundary value problem when (t,x) is given. For the Dirichlet problem, such an algorithm was introduced by Müller [20] and is called the *random walk on spheres*. We are concerned with the heat equation instead of the Laplace equation and, therefore, propose an adaptation of this algorithm in order to consider also the time variable. The algorithm is based on the sequence of random variables $M_n=(T_n,X_n)$ defined by (3.2) and was introduced by Ermakov, Nekruktin and Sipin [7]. The aim of this section is to present the main results of our study: the convergence and the rate of convergence of the algorithm under rather weak conditions on the domain $\mathcal{D}$.

We introduce a stopping rule: let $\varepsilon>0$ be a small parameter, we define $\mathcal{N}_\varepsilon$ the stopping time:

$$\mathcal{N}_\varepsilon:=\inf\big\{n\geq 0:\alpha(T_n,X_n)\leq\varepsilon\big\}, \tag{4.1}$$

where α is given by (3.1):

1. If $\delta^2(X_{\mathcal{N}_\varepsilon},\partial\mathcal{D})\leq\frac{2\varepsilon d}{e}$, then we choose $X_\varepsilon\in\partial\mathcal{D}$ such that
$$\delta(X_{\mathcal{N}_\varepsilon},X_\varepsilon)=\delta(X_{\mathcal{N}_\varepsilon},\partial\mathcal{D})$$
and we denote by $T_\varepsilon:=T_{\mathcal{N}_\varepsilon}$.
2. If $\delta^2(X_{\mathcal{N}_\varepsilon},\partial\mathcal{D})>\frac{2\varepsilon d}{e}$, then we set $T_\varepsilon=0$ and $X_\varepsilon:=X_{\mathcal{N}_\varepsilon}$.

We are now able to give an approximation of the solution to (1.1) by using the definition: for $(t,x)\in[0,T]\times\overline{\mathcal{D}}$,

$$u^{\varepsilon}(t,x)=\mathbb{E}_{(t,x)}\big[f(T_{\varepsilon},X_{\varepsilon})1_{\{X_{\varepsilon}\in\partial\mathcal{D}\}}\big]+\mathbb{E}_{(t,x)}\big[f_0(X_{\varepsilon})1_{\{X_{\varepsilon}\notin\partial\mathcal{D}\}}\big]. \tag{4.2}$$

PROPOSITION 4.1. *Let us assume that the initial-boundary value problem* (1.1) *admits an unique* $\mathcal{C}^{1,2}([0,T]\times\mathcal{D})$*-solution* u*, defined by* (3.3)*. We introduce the approximation* u^{ε} *given by* (4.2)*. Then* u^{ε} *converges towards* u*, as* $\varepsilon\to 0$*, uniformly with respect to* (t,x)*. Moreover, there exist* $\kappa_{T,\mathcal{D}}(u)>0$ *and* $\varepsilon>0$ *such that*

$$\big|u(t,x)-u^{\varepsilon}(t,x)\big|\le\kappa_{T,\mathcal{D}}(u)\sqrt{\varepsilon}\qquad\forall\varepsilon\le\varepsilon_0,(t,x)\in[0,T]\times\mathcal{D}.$$

PROOF. Using the definition of u (resp., u^{ε}) in (3.3) [resp., (4.2)], we obtain

$$\big|u(t,x)-u^{\varepsilon}(t,x)\big|=\big|\mathbb{E}\big[u(T_{\infty},X_{\infty})\big]-\mathbb{E}\big[u(T_{\varepsilon},X_{\varepsilon})\big]\big|.$$

Since $n\mapsto u(T_n,X_n)$ is a bounded martingale and since $\mathcal{N}_{\varepsilon}$ is a finite stopping time (we refer to the proof of Theorem 4.2), we can apply the optimal stopping theorem and the mean value theorem leading to

$$\begin{aligned}\big|u(t,x)-u^{\varepsilon}(t,x)\big|&=\big|\mathbb{E}\big[u(T_{\mathcal{N}_{\varepsilon}},X_{\mathcal{N}_{\varepsilon}})\big]-\mathbb{E}\big[u(T_{\varepsilon},X_{\varepsilon})\big]\big|\\&\le\hat{\kappa}_{T,\mathcal{D}}(u)\mathbb{E}\big[\max\big(|T_{\mathcal{N}_{\varepsilon}}-T_{\varepsilon}|,|X_{\mathcal{N}_{\varepsilon}}-X_{\varepsilon}|\big)\big],\end{aligned}$$

where

$$\hat{\kappa}_{T,\mathcal{D}}(u):=2\sup_{(t,x)\in[0,T]\times\mathcal{D}}\max\left\{\left|\frac{\partial u}{\partial t}(t,x)\right|,\left|\frac{\partial u}{\partial x}(t,x)\right|\right\}.$$

Taking into account the two different situations $\delta^2(X_{\mathcal{N}_{\varepsilon}},\partial\mathcal{D})>\frac{2\varepsilon d}{e}$ or $\delta^2(X_{\mathcal{N}_{\varepsilon}},\partial\mathcal{D})\le\frac{2\varepsilon d}{e}$, we deduce that

$$\max\big(|T_{\mathcal{N}_{\varepsilon}}-T_{\varepsilon}|,|X_{\mathcal{N}_{\varepsilon}}-X_{\varepsilon}|\big)\le\max\left(\varepsilon,\sqrt{\frac{2\varepsilon d}{e}}\right).$$

The statement follows with the particular choice $\kappa_{T,\mathcal{D}}(u)=\hat{\kappa}_{T,\mathcal{D}}(u)\sqrt{\frac{2d}{e}}$. □

Let us now focus our attention on the number of steps needed by the algorithm (3.2) before stopping. In order to present the main result, we need some particular properties on the domain $\mathcal{D}$.

In the sequel, we shall assume that $\mathcal{D}$ is a 0-thick domain (see, for instance, Binder and Bravermann [2]), that is, there exists a constant $C>0$ (so-called the thickness of the domain) such that

$$H^d\big(B(x,r)\setminus\mathcal{D}\big)\ge Cr^d\qquad\forall r<1,\forall x\in\partial\mathcal{D}. \tag{4.3}$$

Here, $H^d(S)$ denotes the d-dimensional Hausdorff content of the set S. This property is namely satisfied by:

- convex domains;
- domains satisfying a cone condition;
- bounded domains with a smooth boundary $\partial\mathcal{D}$.

We observe that the assumption here is quite weak: convergence results associated to random walk type algorithms often require convexity conditions of the domain. Either the domain itself is convex or either it can be split into finitely many convex subdomains. This is namely the case for the walk on spheres algorithm associated with Laplace's equation; we refer to the detailed study of Sabelfeld [24]. Since we just assume that the domain is 0-thick, the usual arguments cannot be used anymore. For such domains, we can prove the following rate of convergence.

THEOREM 4.2. *Let $\mathcal{D} \subset B(0,1)$ be a 0-thick domain. The number of steps $\mathcal{N}_\varepsilon$, of the approximation algorithm, is almost surely finite. Moreover, there exist constants $C > 0$ and $\varepsilon_0 > 0$ such that*

$$\mathbb{E}[\mathcal{N}_\varepsilon] \leq C|\log\varepsilon| \qquad \text{for all } \varepsilon \leq \varepsilon_0. \tag{4.4}$$

The proof of this result is an adaptation of the interesting and recent analysis of the classical random walk on spheres by Binder and Bravermann [2]. Nevertheless, the dynamics of both coordinates of the random walk on spheres $(T_n, X_n)_{n\geq 0}$ being definitively different, this adaptation requires a quite tedious effort. In particular, we need to introduce a particular submartingale, based on the random walk, whose properties permit to prove the rate of convergence.

4.1. *Submartingale related to the Riesz potential.* We consider in this section the 0-thick domain $\mathcal{D}$ which is included in the unit ball of $\mathbb{R}^d$ (assumption of Theorem 4.2). The proof of Theorem 4.2 is based on the so-called Riesz potential. The definition of this particular tool and its first properties essentially depend on the thickness of the domain which plays therefore a crucial role. We introduce the set $\mathcal{M}$ of all Borel measures μ supported inside $\overline{B(0,2)}$ and outside of $\mathcal{D}$, satisfying the following condition:

$$\mu\big(B(x,r)\big) \leq r^d \qquad \forall x \in \mathbb{R}^d, \forall r > 0. \tag{4.5}$$

Let us define the so-called *energy function* U:

$$U(x) = \sup_{\mu\in\mathcal{M}} U^\mu(x),$$

where U^μ stands for the Riesz potential of the measure μ, that is,

$$U^\mu(x) = \int_0^\infty \frac{\mu(B(x,r))}{r^{d+1}}\,\mathrm{d}r. \tag{4.6}$$

Both the choice of the particular set of measures $\mathcal{M}$ and the expression of the Riesz potential are related to the thickness of the domain. The definition of U obviously implies that $U(x) \geq 0$ for any $x \in \mathbb{R}^d$.

REMARK 4.3. Binder and Bravermann [2] gave several properties of this energy function. We just recall some of them:

1. Since the set of measures $\mathcal{M}$ is weakly*-compact, there exists a family of measures μ_x, belonging to $\mathcal{M}$, such that $U(x) = U^{\mu_x}(x)$. This property will play a crucial role in the proof of Proposition B.2.

2. The energy function U is subharmonic in $\mathcal{D}$. Consequently, due to the construction of the random walk (T_n, X_n), which is based on uniform random variables on moving spheres, the process $(U(X_n))_{n\geq 0}$ is a submartingale with respect to the filtration generated by $(T_n, X_n)_{n\geq 0}$:

$$\mathcal{F}_n := \sigma\{T_1, \ldots, T_n, X_1, \ldots, X_n\}.$$

Hence

$$\mathbb{E}\big[U(X_{n+1})|\mathcal{F}_n\big] \geq U(X_n) \qquad \text{a.s.} \tag{4.7}$$

3. Easy computations on the Riesz potential permits to prove that

$$U(x) \leq \log \frac{3}{\delta(x, \partial\mathcal{D})} + \frac{1}{d} \qquad \forall x \in \mathcal{D}. \tag{4.8}$$

This inequality requires that the thickness of the domain is smaller than 2 and differs from the space dimension. In particular, we obtain an important property of the submartingale $(U(X_n))_{n\geq 0}$:

$$\text{If } U(X_n) \geq \log \frac{3}{\varepsilon} + \frac{1}{d} \qquad \text{then } \delta(X_n, \mathcal{D}) \leq \varepsilon. \tag{4.9}$$

These properties, of the energy function U, permit to sketch the proof of the convergence in the classical random walk on spheres case. Indeed we know that $U(X_n)$ is a submartingale and the algorithm stops before $U(X_n)$ becomes too large. So, it suffices to focus the attention on the time needed by the submartingale to exceed some given large threshold.

In the algorithm described by (3.2), a large value of $U(X_n)$ is not sufficient to ensure that the stopping rule has been reached. Indeed the stopping procedure depends on both space and time variables, through the condition: $\alpha(T_n, X_n) \leq \varepsilon$. That is why we need to adapt the classical study by considering a martingale based on the Riesz potential but taking also into account the decreasing time sequence $(T_n)_{n\geq 0}$.

Let us define the *modified energy function* on $\mathbb{R}_+ \times \mathbb{R}^d$ by

$$\mathbb{U}(t, x) = \max\left\{\frac{1}{2}\log\left(\frac{3}{t}\right), U(x)\right\}. \tag{4.10}$$

This function will play a similar role as the energy function (in the classical case). In particular, if we apply $\mathbb{U}$ to the sequence (T_n, X_n), we obtain a submartingale with nice properties.

LEMMA 4.4. *We define* $\mathbb{U}_n := \mathbb{U}(T_n, X_n)$. *Then the process* $(\mathbb{U}_n)_{n\geq 0}$ *is a* $\mathcal{F}$*-submartingale.*

PROOF. First, we can notice that

$$T_{n+k} \leq T_n \quad \Rightarrow \quad \log \frac{3}{T_{n+k}} \geq \log \frac{3}{T_n}.$$

By Jensen's inequality (see Lemma A.1) and using the submartingale property (4.7) of $U(X_n)$, we obtain

$$\begin{aligned}
\mathbb{E}\big[\mathbb{U}_{n+1}|\sigma(T_n, X_n)\big] &= \mathbb{E}\bigg[\max\bigg\{\frac{1}{2}\log\frac{3}{T_{n+1}}, U(X_{n+1})\bigg\}\Big|\sigma(T_n, X_n)\bigg] \\
&\geq \mathbb{E}\bigg[\max\bigg\{\frac{1}{2}\log\frac{3}{T_n}, U(X_{n+1})\bigg\}\Big|\sigma(T_n, X_n)\bigg] \\
&\geq \max\bigg\{\frac{1}{2}\log\frac{3}{T_n}, \mathbb{E}\big[U(X_{n+1})|\sigma(T_n, X_n)\big]\bigg\} \\
&\geq \max\bigg\{\frac{1}{2}\log\frac{3}{T_n}, U(X_n)\bigg\} = \mathbb{U}_n.
\end{aligned}$$

We deduce that $(\mathbb{U}_n)$ is a submartingale as announced. □

In order to describe an upper-bound for the sequence $\mathbb{E}[\mathbb{U}_n^2]$, we first point out an inequality relating $\mathbb{U}(t, x)$ to the function $\alpha(t, x)$, which plays an essential role in the algorithm (3.2).

LEMMA 4.5. *There exists a constant* $\kappa > 0$ (*depending only on the space dimension* d) *such that*

$$\mathbb{U}(t, x) \leq \kappa - \frac{1}{2}\log\big(\alpha(t, x)\big) \qquad \forall (t, x) \in \mathbb{R}_+ \times \mathcal{D}. \tag{4.11}$$

PROOF. On one hand, the definition of $\alpha(t, x)$ in equation (3.1) implies that $\frac{e}{2d}\delta^2(x, \partial\mathcal{D}) \geq \alpha(t, x)$, and consequently

$$\log\frac{3}{\delta(x, \partial\mathcal{D})} \leq \frac{1}{2}\log\frac{9e}{2d} - \frac{1}{2}\log\alpha(t, x).$$

Using the property (4.8), we obtain

$$U(x) \leq -\frac{1}{2}\log\alpha(t, x) + \frac{1}{2}\log\frac{9e}{2d} + \frac{1}{d}.$$

On the other hand, the definition of $\alpha(t, x)$ also implies

$$\frac{1}{2}\log\frac{3}{t} \leq \frac{1}{2}\log\frac{3}{\alpha(t, x)} = \frac{\log 3}{2} - \frac{1}{2}\log\alpha(t, x).$$

Combining both inequalities, we deduce that $\mathbb{U}(t,x) = \max\{\frac{1}{2}\log(3/t), U(x)\}$ satisfies (4.11) with $\kappa := \max\{\frac{1}{2}\log 3, \frac{1}{2}\log\frac{9e}{2d} + \frac{1}{d}\}$. $\square$

An immediate consequence of Lemma 4.5 is an L^2-bound of $\mathbb{U}_n$, n fixed.

PROPOSITION 4.6. *Let $(T_0, X_0) = (t,x)$. There exist two constants C_1 and C_2 such that*

$$\mathbb{E}[\mathbb{U}_n^2] \le (C_1 + C_2 n)^2 \qquad \text{for } n \ge \kappa - \frac{1}{2}\log\big(\alpha(t,x)\big).$$

Here, κ stands for the constant defined in Lemma 4.5.

PROOF. Let us first recall that $\mathbb{U}_n := \mathbb{U}(T_n, X_n)$. Due to the definition of the function U, we observe that $U(x) \ge 0$ for any $x \in \mathbb{R}^d$, and consequently $\mathbb{U}(t,x) \ge 0$ and $\mathbb{U}_n \ge 0$. Due to Lemma 4.5, we shall focus our attention on $\log\alpha(T_n, X_n)$.

First, we notice that (3.2) leads to

$$T_n = T_{n-1} - \alpha(T_{n-1}, X_{n-1})R_n \ge T_{n-1}(1 - R_n).$$

Hence

$$\begin{aligned} -\log(T_n) &\le -\log(T_{n-1}) - \log(1 - R_n) \\ &\le -\log\big(\alpha(T_{n-1}, X_{n-1})\big) - \log(1 - R_n). \end{aligned} \tag{4.12}$$

Moreover, by (3.2),

$$\delta(X_n, \partial\mathcal{D}) \ge \delta(X_{n-1}, \partial\mathcal{D}) - 2\sqrt{\alpha(T_{n-1}, X_{n-1})}\psi(R_n).$$

By its definition, $\alpha(t,x) \le \frac{e}{2d}\delta^2(x, \partial\mathcal{D})$, and we obtain

$$\delta(X_n, \partial\mathcal{D}) \ge \delta(X_{n-1}, \partial\mathcal{D})\left(1 - \sqrt{\frac{2e}{d}}\psi(R_n)\right),$$

and, therefore,

$$\begin{aligned} &-\log\left(\frac{e}{2d}\delta^2(X_n, \partial\mathcal{D})\right) \\ &\quad\le -\log\big(\alpha(T_{n-1}, X_{n-1})\big) - 2\log\left(1 - \sqrt{\frac{2e}{d}}\psi(R_n)\right). \end{aligned} \tag{4.13}$$

Let us define $W_n := -2\log(1 - \sqrt{\frac{2e}{d}}\psi(R_n)) - \log(1 - R_n)$. Combining (4.12) and (4.13), we finally obtain

$$\begin{aligned} -\log\big(\alpha(T_n, X_n)\big) &\le -\log\big(\alpha(T_{n-1}, X_{n-1})\big) + W_n \\ &\le -\log\big(\alpha(t,x)\big) + \sum_{k=1}^{n} W_k. \end{aligned} \tag{4.14}$$

Let us just note that (W_n) is a family of independent and identically distributed random variables and (t,x) is the starting position of the algorithm. Let us recall that $\mathbb{U}_n \geq 0$. We obtain

$$\begin{aligned}
\mathbb{E}[\mathbb{U}_n^2] &\leq \mathbb{E}\left[\left(\kappa - \frac{1}{2}\log(\alpha(T_n, X_n))\right)^2\right] \\
&\leq \mathbb{E}\left[\left(\kappa - \frac{1}{2}\log(\alpha(T_0, X_0)) + \sum_{k=1}^{n} W_k\right)^2\right] \\
&\leq 2\left(\kappa - \frac{1}{2}\log(\alpha(t,x))\right)^2 + 2\mathbb{E}\left[\left(\sum_{k=1}^{n} W_k\right)^2\right] \\
&\leq 2\left(\kappa - \frac{1}{2}\log(\alpha(t,x))\right)^2 + 2\operatorname{Var}\left(\sum_{k=1}^{n} W_k\right) + 2\mathbb{E}\left[\sum_{k=1}^{n} W_k\right]^2 \\
&\leq 2\left(\kappa - \frac{1}{2}\log(\alpha(t,x))\right)^2 + 2n\operatorname{Var}(W_1) + 2n^2\big(\mathbb{E}[W_1]\big)^2 \\
&\leq 2n\operatorname{Var}(W_1) + 2n^2\big(\mathbb{E}[W_1]^2 + 1\big),
\end{aligned}$$

due to the hypothesis $n \geq \kappa - \frac{1}{2}\log(\alpha(t,x))$. So Lemma A.2 implies the statement of the Proposition 4.6: the upper-bound is quadratic with respect to n. □

Let us now point out a lower-bound for the expected value of the submartingale: $(\mathbb{E}[\mathbb{U}_n])_{n\geq 0}$.

PROPOSITION 4.7. *There exist two constants $C_3 \in \mathbb{R}$ and $C_4 > 0$, such that*

$$\mathbb{E}[\mathbb{U}_n] \geq C_3 + C_4 n, \qquad n \geq 1. \tag{4.15}$$

PROOF. Since $(\mathbb{U}_n)_{n\geq 0}$ is a submartingale, we know that $(\mathbb{E}[\mathbb{U}_n])_{n\geq 0}$ is a non-decreasing sequence, but we need even more. In fact, due to the following lower-bound:

$$\mathbb{U}_n \geq \frac{1}{4}\log\frac{3}{T_n} + \frac{1}{2}U(X_n) =: \mathbb{V}_n,$$

it suffices to point out the existence of a constant $L_0 > 0$ such that

$$\mathbb{E}[\mathbb{V}_{n+1}] - \mathbb{E}[\mathbb{V}_n] \geq L_0 \qquad \forall n \geq 0. \tag{4.16}$$

In order to compute such a lower-bound, we consider two cases: either $\alpha(T_n, X_n) = T_n$ (event denoted by $\mathcal{T}_n$) or $\alpha(T_n, X_n) \neq T_n$ (event denoted by $\overline{\mathcal{T}}_n$).

Step 1. $\alpha(T_n, X_n) = T_n$. Then the definition of the random walk (3.2) implies that

$$T_{n+1} = T_n - \alpha(T_n, X_n)R_{n+1} = T_n(1 - R_{n+1}) \qquad \text{on } \mathcal{T}_n.$$

Hence

$$\log \frac{3}{T_{n+1}} = \log \frac{3}{T_n} - \log(1 - R_{n+1}) \qquad \text{on } \mathcal{T}_n.$$

Let us denote by $L_1 = -\frac{1}{4}\mathbb{E}[\log(1 - R_1)] > 0$. Since $U(X_n)$ is a submartingale (U being subharmonic in $\mathcal{D}$), we get

$$\begin{aligned}
\mathbb{E}[\mathbb{V}_{n+1} 1_{\mathcal{T}_n}] &= \mathbb{E}\Big[\frac{1}{4}\log\frac{3}{T_{n+1}} 1_{\mathcal{T}_n}\Big] + \frac{1}{2}\mathbb{E}\big[\mathbb{E}\big[U(X_{n+1})|\mathcal{F}_n\big] 1_{\mathcal{T}_n}\big] \\
&\geq \mathbb{E}\Big[\frac{1}{4}\log\frac{3}{T_n} 1_{\mathcal{T}_n}\Big] + L_1 \mathbb{P}(\mathcal{T}_n) + \frac{1}{2}\mathbb{E}\big[U(X_n) 1_{\mathcal{T}_n}\big] \\
&\geq \mathbb{E}[\mathbb{V}_n 1_{\mathcal{T}_n}] + L_1 \mathbb{P}(\mathcal{T}_n). \qquad (4.17)
\end{aligned}$$

Step 2. $\alpha(T_n, X_n) \neq T_n$. Let us recall that the random walk satisfies: $X_{n+1} = X_n + 2\sqrt{\alpha(T_n, X_n)}\psi_d(R_{n+1})V_{n+1}$ where R_{n+1} is a continuous random variable whose support is the whole interval $[0, 1]$ and whose distribution does not depend on n. Observe also that

$$\rho(R_{n+1}) := \sqrt{\frac{2e}{d}}\psi_d(R_{n+1})$$

is a continuous random variable with support $[0, 1]$. In other words, on the event $\alpha(T_n, X_n) \neq T_n$ and given $R_{n+1} = r$, the $(n+1)$th step of the random walk is exactly the same as the $(n+1)$th step of the classical random walk on spheres (see Appendix B) with radius $\beta = \rho(r)$, for which we can obtain some lower-bound. So using Proposition B.2, we obtain

$$\begin{aligned}
\mathbb{E}[\mathbb{V}_{n+1} 1_{\overline{\mathcal{T}}_n}] &= \mathbb{E}\Big[\frac{1}{4}\log\frac{3}{T_{n+1}} 1_{\overline{\mathcal{T}}_n}\Big] + \frac{1}{2}\mathbb{E}\big[U(X_{n+1}) 1_{\overline{\mathcal{T}}_n}\big] \\
&\geq \mathbb{E}\Big[\frac{1}{4}\log\frac{3}{T_n} 1_{\overline{\mathcal{T}}_n}\Big] + \frac{1}{2}\mathbb{E}\big[\mathbb{E}\big[U(X_{n+1})|\sigma(R_{n+1}, T_n, X_n)\big] 1_{\overline{\mathcal{T}}_n}\big] \\
&\geq \mathbb{E}\Big[\frac{1}{4}\log\frac{3}{T_n} 1_{\overline{\mathcal{T}}_n}\Big] + \frac{1}{2}\mathbb{E}\big[\big(U(X_n) + L 1_{\{\delta/4 < 1 - \rho(R_{n+1}) < \delta/2\}}\big) 1_{\overline{\mathcal{T}}_n}\big] \\
&\geq \mathbb{E}[\mathbb{V}_n 1_{\overline{\mathcal{T}}_n}] + \frac{L}{2}\mathbb{P}\big(\{\delta/4 < 1 - \rho(R_{n+1}) < \delta/2\} \cap \overline{\mathcal{T}}_n\big) \qquad (4.18) \\
&= \mathbb{E}[\mathbb{V}_n 1_{\overline{\mathcal{T}}_n}] + L_2 \mathbb{P}(\overline{\mathcal{T}}_n), \qquad (4.19)
\end{aligned}$$

where $L_2 = \frac{L}{2}\mathbb{P}(\delta/4 < 1 - \rho(R_1) < \delta/2)$, R_{n+1} and (T_n, X_n) being independent. Finally, taking the sum of (4.17) and (4.18), we obtain (4.16) with $L_0 = \min(L_1, L_2) > 0$. □

We end here the preliminary results concerning the submartingale $(\mathbb{U}_n)_{n\geq 0}$. We are now ready to deal with the rate of convergence of the random walk on moving spheres.

4.2. *Rate of convergence of the algorithm.* Let us consider the algorithm $(T_n, X_n)_{n\geq 0}$ given by (3.2) and stopped as soon as $\alpha(T_n, X_n) \leq \varepsilon$. We assume that the starting position satisfies $(T_0, X_0) = (t, x) \in \mathbb{R}_+ \times \mathcal{D}$. Then the mean number of steps is bounded and the bound depends on $|\log \varepsilon|$.

PROOF OF THEOREM 4.2. If the starting position (t, x) satisfies $\alpha(t, x) \leq \varepsilon$, then the algorithm stops immediately ($\mathcal{N}_\varepsilon = 0$ a.s.) and the statement is satisfied. From now on, we assume that $\alpha(t, x) > \varepsilon$.

Step 1. A remark on the stopping rule. The statement of Theorem 4.2 concerns $\mathcal{N}_\varepsilon$ [see (4.1)] the first time the random walk $(T_n, X_n)_{n\geq 0}$ hits a ε-neighborhood of the boundary. Let us introduce another stopping rule concerning $\mathbb{U}_n := \mathbb{U}(T_n, X_n)$, $\mathbb{U}$ being defined by (4.10):

$$\mathcal{N}'_\varepsilon := \inf\left\{n \geq 0 : \mathbb{U}_n \geq \log\frac{3}{\varepsilon} + \frac{1}{d}\right\}.$$

Let us now point out that $\mathcal{N}_\varepsilon \leq \mathcal{N}'_\varepsilon$ a.s. for ε small enough (more precisely, we need $\varepsilon \leq \frac{2d}{e}$).

Indeed, let us consider the first case: $U(X_n) \geq \log\frac{3}{\varepsilon} + \frac{1}{d}$, then (4.9) implies that $\delta(X_n, \partial\mathcal{D}) \leq \varepsilon$. Moreover, due to the condition $\varepsilon \leq \frac{2d}{e}$, we get $\frac{e}{2d}\delta^2(X_n, \partial\mathcal{D}) \leq \varepsilon$ and, therefore, $\alpha(T_n, X_n) \leq \varepsilon$.

On the other side, if $\frac{1}{2}\log\frac{3}{T_n} \geq \log\frac{3}{\varepsilon} + \frac{1}{d} \geq \frac{1}{2}\log\frac{3}{\varepsilon}$ then $T_n \leq \varepsilon$, and finally $\alpha(T_n, X_n) \leq \varepsilon$. So we deduce that $\mathbb{U}_n \geq \log\frac{3}{\varepsilon} + \frac{1}{d}$ implies that $\alpha(T_n, X_n) \leq \varepsilon$. In the sequel, we will find an upper-bound for the mean value of $\mathcal{N}'_\varepsilon$.

Step 2. The aim of the second step is to prove the existence of an integer $\eta \in \mathbb{N}$ and a constant $p < 1$ both independent with respect to the starting position of the random walk $(T_0, X_0) = (t, x)$ and independent of the parameter ε such that

$$\mathbb{P}\big(\mathcal{N}'_\varepsilon > \eta\lfloor -\log\varepsilon\rfloor\big) \leq p \tag{4.20}$$

for ε small enough. Let us note that the complementary event satisfies, by definition,

$$\mathbb{P}\big(\mathcal{N}'_\varepsilon \leq \eta\lfloor -\log\varepsilon\rfloor\big) \geq \mathbb{P}(\mathbb{U}_k \geq \beta_k),$$

where $k = \eta\lfloor -\log\varepsilon\rfloor$ and $\beta_k = \log 3 + 1 + \frac{1}{d} + k/\eta$. We deduce that there exists a particular choice of the integer η such that, for ε small enough, $\beta_k < \alpha_k := (C_3 + C_4 k)/2$ where C_3 and C_4 are defined in Proposition 4.7. So it is sufficient to find a lower-bound of $\mathbb{P}(\mathbb{U}_k > \alpha_k)$ which should be positive when k is large. By Proposition 4.6, there exist two constants C_1 and C_2 such that

$$\mathbb{E}\big[\mathbb{U}_n^2\big] \leq (C_1 + C_2 n)^2 \qquad \text{for any } n \geq \kappa - \frac{1}{2}\log\big(\alpha(t, x)\big).$$

Due to the condition on the initial position $\alpha(t, x) > \varepsilon$, the previous inequality is satisfied for $n \geq \lfloor -\log\varepsilon\rfloor$ when ε is small enough. In particular, it is satisfied for

$n = k = \eta\lfloor -\log\varepsilon\rfloor$. We obtain

$$\mathbb{E}[\mathbb{U}_k] = \mathbb{E}[\mathbb{U}_k 1_{\{\mathbb{U}_k \le \alpha_k\}}] + \mathbb{E}[\mathbb{U}_k 1_{\{\mathbb{U}_k > \alpha_k\}}] > C_3 + C_4 k. \tag{4.21}$$

Then by an application of (4.15) and the Cauchy–Schwarz inequality, we get

$$\alpha_k + \sqrt{\mathbb{E}[\mathbb{U}_k^2]}\sqrt{\mathbb{P}(\mathbb{U}_k > \alpha_k)} > C_3 + C_4 k.$$

Therefore, due to the upper-bound of the second moment,

$$\alpha_k + (C_1 + C_2 k)\sqrt{\mathbb{P}(\mathbb{U}_k > \alpha_k)} > C_3 + C_4 k.$$

We deduce

$$\mathbb{P}(\mathbb{U}_k > \alpha_k) \ge \frac{1}{4}\left(\frac{C_3 + C_4 k}{C_1 + C_2 k}\right)^2 > \frac{1}{5}\left(\frac{C_4}{C_2}\right)^2$$

for k large enough that is ε small enough. This implies the existence of the constant $p > 0$ in (4.20).

Step 3. Upper-bound of $\mathbb{E}[\mathcal{N}'_\varepsilon]$. Due to the first step it is sufficient to obtain an upper-bound of $\mathbb{E}[\mathcal{N}'_\varepsilon]$ in order to prove the statement of the theorem. Such a result is essentially based on the Markov property of the sequence $(T_n, X_n)_{n\ge 0}$: the second step implies in particular that

$$\mathbb{P}\big(\mathcal{N}'_\varepsilon > k\eta\lfloor -\log\varepsilon\rfloor\big) \le p^k \qquad \forall k \ge 1.$$

Hence

$$\begin{aligned}\mathbb{E}[\mathcal{N}'_\varepsilon] &\le \sum_{k\ge 1} k\eta\lfloor -\log\varepsilon\rfloor \mathbb{P}\big(\mathcal{N}'_\varepsilon \le k\eta\lfloor -\log\varepsilon\rfloor | \mathcal{N}'_\varepsilon > (k-1)\eta\lfloor -\log\varepsilon\rfloor\big) \\ &\quad \times \mathbb{P}\big(\mathcal{N}'_\varepsilon > (k-1)\eta\lfloor -\log\varepsilon\rfloor\big) \\ &\le \eta\lfloor -\log\varepsilon\rfloor \sum_{k\ge 1} k p^{k-1} = \frac{\eta|\log\varepsilon|}{(1-p)^2},\end{aligned}$$

and thus obtaining the desired upper-bound. □

5. Examples and numerics. The aim of this section is to illustrate the random walk on spheres algorithm introduced in Section 4. Let us focus our attention on the numerical approximation of the solution to the value problem:

$$\begin{cases} \partial_t u(t,x) - \Delta_x u(t,x) = 0 & \forall (t,x) \in \mathbb{R}_+ \times \mathcal{D}, \\ u(t,x) = f(t,x) & \forall (t,x) \in \mathbb{R}_+ \times \partial\mathcal{D}, \\ u(0,x) = f_0(x) & \forall x \in \mathcal{D} \end{cases} \tag{5.1}$$

for particular domains $\mathcal{D}$. First, we shall present results obtained for the hypercube $\mathcal{D} =]0, L[^d$, $L > 0$, and second, the half of a sphere

$$\mathcal{D} = \big\{x \in \mathbb{R}^d : \|x\| < 1, x_1 > 0\big\}.$$

Of course, these toy examples are not directly related to concrete situations in physics but they permit to emphasize the efficiency of the algorithm. Their advantage relies in the easy computation of the distance to the boundary. For more general situations, only this part of the procedure has to be modified and can in some cases become difficult to implement and especially time-consuming.

5.1. *Hypercube.* Let us first introduce the functions related to the boundary conditions. We choose a function with the following simple expression:

$$f(t,x) = e^{-d\pi^2 t/L} \prod_{i=1}^{d} \sin\left(\pi x_i / L^2\right), \qquad x \in \overline{\mathcal{D}}, \forall t \geq 0. \tag{5.2}$$

Setting $f_0(x) = f(0,x)$, we observe that both the compatibility and the continuity conditions are obviously satisfied. In this particular case, we have already pointed out, in the previous sections, that there exists a unique (smooth) solution to the initial-boundary value problem which can be approximated using the algorithm of moving spheres. The choice of the function (5.2) is particularly convenient since the IBVP solution is explicitly known: $u(t,x) = f(t,x)$ which permit to compare in an efficient way the exact and the approximated solutions.

The solution can be approximated by u^ε defined by (4.2), the error being directly related to the parameter ε. Since $u^\varepsilon(t,x)$ is the expectation of a random variable, we shall use a Monte Carlo method in order to obtain an estimated value. Hence

$$u_N^\varepsilon(t,x) = \frac{1}{N}\sum_{k=1}^{N} f(T_{\varepsilon,k}, X_{\varepsilon,k}) 1_{\{X_{\varepsilon,k}\in\partial\mathcal{D}\}} + \frac{1}{N}\sum_{k=1}^{N} f_0(X_{\varepsilon,k}) 1_{\{X_{\varepsilon,k}\notin\partial\mathcal{D}\}}, \tag{5.3}$$

where $(T_{\varepsilon,k}, X_{\varepsilon,k})_{k\geq 0}$ is a sequence of independent and identically distributed couples of random variables, the distribution being defined at the beginning of Section 4. The difference between $u(t,x)$ and $u_N^\varepsilon(t,x)$ actually relies on both the error described in Proposition 4.1 of order $\sqrt{\varepsilon}$ on one hand and the classical error of Monte Carlo methods of order $N^{-1/2}$ on the other hand (the confidence interval depends as usual on the standard deviation of the underlying random variable).

First, let us present $u_N^\varepsilon(t,x)$ for a particular point: the center of the hypercube [$x = (L/2, \ldots, L/2)$ is the default setting in all this subsection] letting the time cross the whole interval $[0,2]$.

We present at the same time the associated Monte Carlo 95%-confidence interval (Figure 3). Let us just notice that the choice $N = 1000$ is not motivated by some computational facilities but rather to produce a clear picture, the confidence interval becoming very small for larger values of N. Of course, the numerical method permits to observe directly the distribution of the random variable

$$\mathcal{Z}_\varepsilon = f(T_\varepsilon, X_\varepsilon) 1_{\{X_\varepsilon\in\partial\mathcal{D}\}} + f_0(X_\varepsilon) 1_{\{X_{\varepsilon,k}\notin\partial\mathcal{D}\}},$$

which drastically changes as time elapses (Figures 4 and 5).

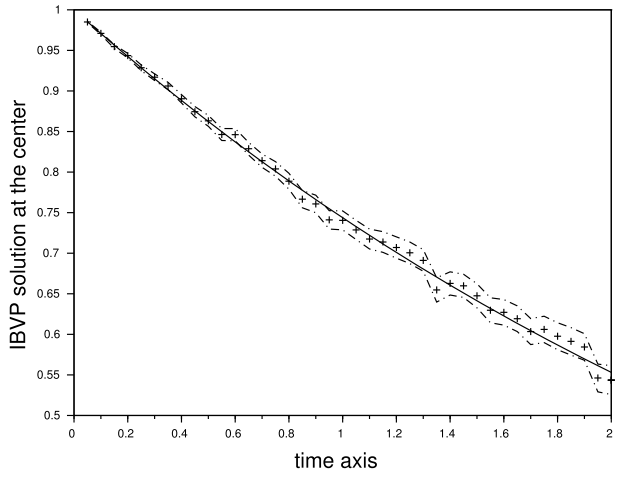

FIG. 3. *IBVP solution versus t. The figure presents the exact solution* (*solid line*), *the approximated solution* $u_N^{\varepsilon}(t,x)$ (*plus sign*) *and its Monte Carlo* 95%*-confidence interval*, *for x the center of the hypercube*, $L = 10$, $N = 1000$, $\varepsilon = 0.001$, $d = 3$.

In our example, small values of $\mathcal{Z}_\varepsilon$ are more frequently observed for small time values than for large ones. Such behaviour of the random variable is not linked to the particular boundary conditions we introduced, but relies on the following general argument. The random variable $\mathcal{Z}_\varepsilon$ is obtained due to a stopping procedure on $M_n = (T_n, X_n)$ defined by (3.2). The sequence is stopped as soon as either X_n is ε-close to the boundary $\partial\mathcal{D}$ (we call this event *stop due to space constraint*) or T_n is ε-close to 0 (*stop due to time constraint*). Then it seems quite obvious that stops due to time constraint are more likely to occur when t becomes small [see the proportion in Figure 6(left)].

Let us now comment the algorithm efficiency by focusing our attention on the number of steps. The distribution of this random number depends on several parameters: the dimension d, the parameter ε, and finally the choice of (t,x) [see

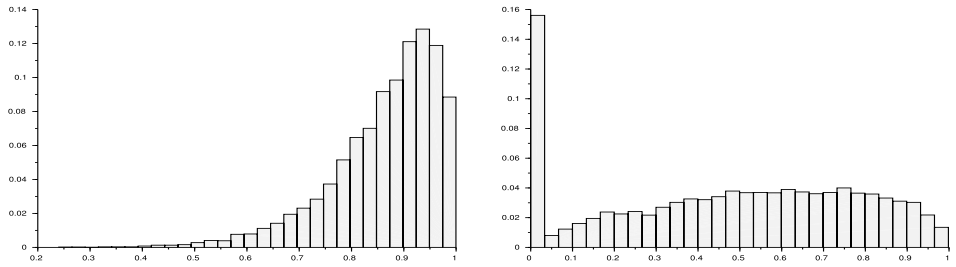

FIG. 4. *Histogram of the distribution of* 10,000 *random variables* $\mathcal{Z}_\varepsilon$ *for various values of t*: $t = 0.5$ (*left*), $t = 2.5$ (*right*), $\varepsilon = 0.001$, $L = 5$, $d = 3$.

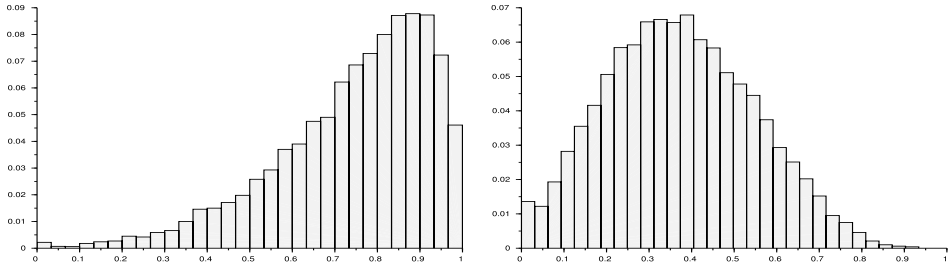

FIG. 5. *Histogram of $\mathcal{Z}_\varepsilon$ for $d = 3$ (left) and $d = 10$ (right), $t = 1$, $\varepsilon = 0.001$.*

histogram Figure 6(right) for a particular choice of parameters]. We have pointed out an upper bound for the average number of steps in Theorem 4.2. The numerics permit to present different curves illustrating all the dependences: the logarithm growth with respect to the parameter ε, the behavior when the space position x varies and the influence of the dimension (Figures 7 and 8). Let us notice that this algorithm is especially efficient (see the small number of steps) even in high dimensions.

5.2. *Half-sphere.* All the studies developed in the hypercube case can also be considered for the half-sphere. We introduce particular boundary conditions:

$$f(t,x) = \big(1 + \cos(2\pi t)\big)\|x\| \qquad \forall x \in \overline{\mathcal{D}}, \forall t \geq 0, \tag{5.4}$$

with $f_0(x) = f(0,x)$. Similarly, as above, we present:

- the approximated solution $u_N^\varepsilon(t,x)$ and its Monte Carlo 95%-confidence interval, for the default value $x = (0.5, 0, \ldots, 0)$ and for t varying in the interval $[0, 2]$ (Figure 9),

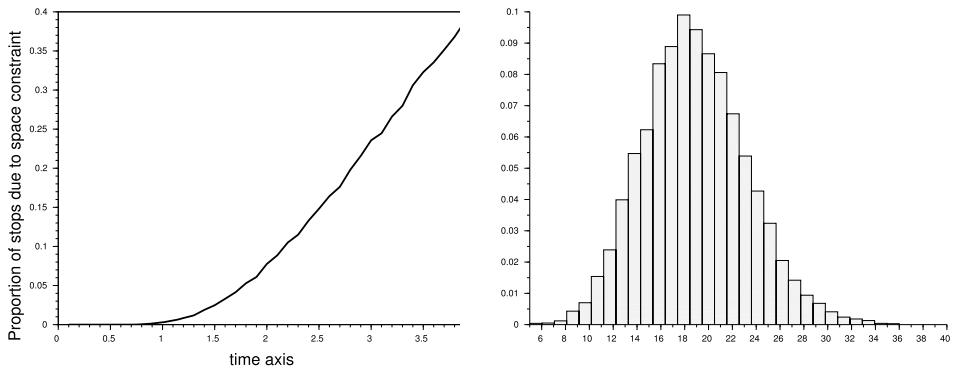

FIG. 6. *Proportion of stops due to space constraint versus t for* 10,000 *trials*, $\varepsilon = 0.001$, $d = 3$ (*left*); *histogram of the number of steps* $t = 1$, $\varepsilon = 0.001$, $d = 3$.

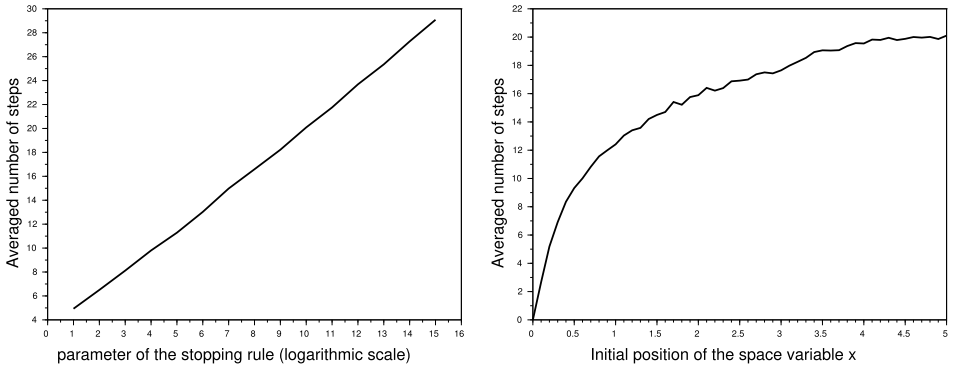

FIG. 7. *Averaged number of steps versus n for* $\varepsilon = 0.5^n$ *and x the center of the hypercube* (*left*), *averaged number of steps versus u for* $x = (u, u, u)$ *and* $\varepsilon = 0.001$. *In both situations*: 10,000 *trials*, $d = 3$, $t = 4$.

- the distribution of the Monte Carlo underlying variable $\mathcal{Z}^{\varepsilon}$ for different values of t and different dimension values d (Figures 10 and 11),
- different curves illustrating the influence of the parameter ε, the starting position x and the dimension d on the averaged number of steps (Figures 12 and 13).

APPENDIX A: TECHNICAL RESULTS

We first start with Jensen's inequality:

LEMMA A.1. *Let X and Y be two random variables and* $\mathcal{A}$ *a* σ*-algebra, then the following inequalities hold*: $\mathbb{E}[\max(X, Y)] \geq \max(\mathbb{E}[X], \mathbb{E}[Y])$ *and* $\mathbb{E}[\max(X, Y)|\mathcal{A}] \geq \max(\mathbb{E}[X|\mathcal{A}], \mathbb{E}[Y|\mathcal{A}])$.

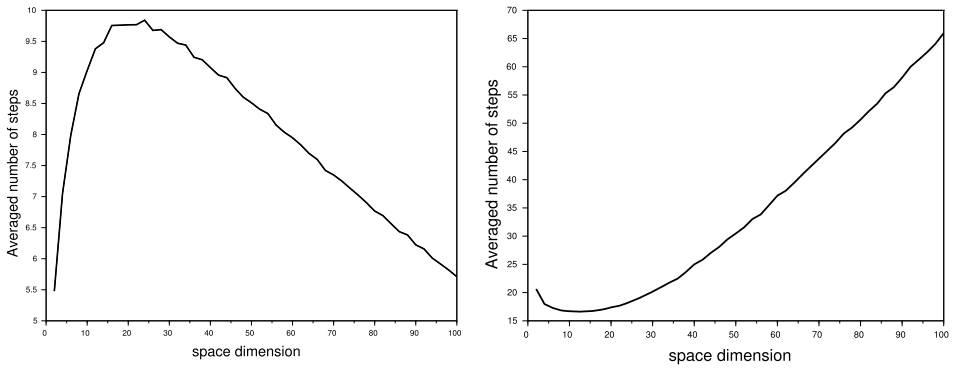

FIG. 8. *Averaged number of steps versus the dimension d*, $\varepsilon = 0.001$, 10,000 *trials*, $t = 4$. *The left graph concerns the hypercube of side length* $L = 1$ *while the right one corresponds to* $L = 10$. *For both of them, the algorithm starts at the center of the hypercube.*

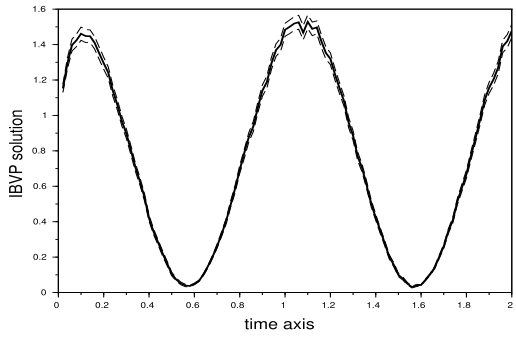

FIG. 9. *The value of the IBVP approximated solution* $u_N^{\varepsilon}(t,x)$ *versus* t *for* $N = 1000$, $\varepsilon = 0.001$, $d = 3$.

PROOF. We shall just prove the first inequality. The proof of the second one is similar. We get

$$\mathbb{E}\big[\max(X,Y)\big] = \mathbb{E}\big[\mathbb{E}\big[\max(X,Y)|X\big]\big] \geq \mathbb{E}\big[\max\big(X,\mathbb{E}[Y|X]\big)\big].$$

Since $\max(X,\mathbb{E}[Y|X]) \geq X$, we deduce that $\mathbb{E}[\max(X,\mathbb{E}[Y|X])] \geq \mathbb{E}[X]$. On the other side $\max(X,\mathbb{E}[Y|X]) \geq \mathbb{E}[Y|X]$ and, therefore, $\mathbb{E}[\max(X,\mathbb{E}[Y|X])] \geq \mathbb{E}[\mathbb{E}[Y|X]] = \mathbb{E}[Y]$. Combining both inequalities leads to the result. □

Let us now present properties concerning a particular probability distribution arising in the random walk on moving spheres.

LEMMA A.2. *Let* $W := -2\log(1-\sqrt{\frac{2e}{d}}\psi_d(R)) - \log(1-R)$ *where the function* ψ_d *is defined by* (2.3) *and* R *is a random variable with the following probability density function*:

$$f_R(s) = \frac{1}{\Gamma(d/2)}\frac{\psi_d^d(s)}{s}1_{[0,1]}(s) = \frac{1}{s\Gamma(d/2)}\big(s\log\big(s^{-d/2}\big)\big)^{d/2}1_{[0,1]}(s).$$

Then W *has its two first moments* (*denoted by* $\mathcal{M}_1$ *and* $\mathcal{M}_2$) *bounded.*

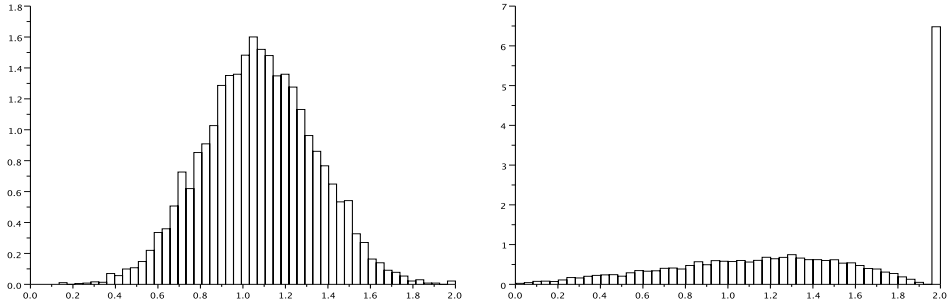

FIG. 10. *Histogram of the distribution of* 10,000 *random variables* $\mathcal{Z}_\varepsilon$ *for various values of* t: $t = 0.01$ (*left*), $t = 0.05$ (*right*), *both with* $\varepsilon = 0.001$, $d = 3$ *and* $x = (0.5, 0, 0)$.

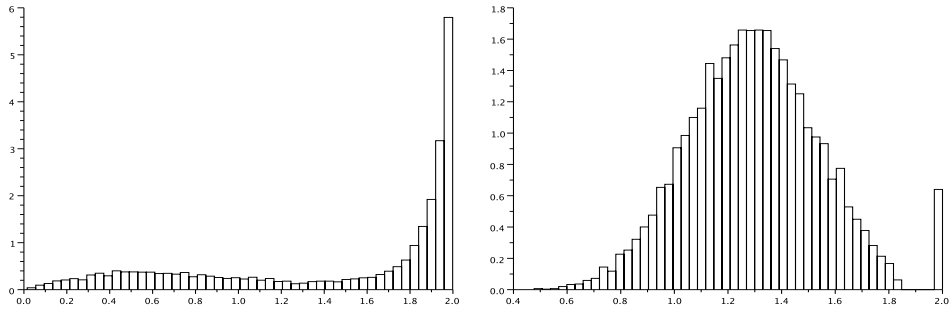

FIG. 11. *Histogram of $\mathcal{Z}_\varepsilon$ for $d = 3$ and $t = 1$ (left), for $d = 10$ and $t = 0.01$ (right), both with $\varepsilon = 0.001$ and $x = (0.5, 0, 0)$.*

PROOF. Let us first note that W is a nonnegative random variable, since R and $\sqrt{\frac{2e}{d}}\psi_d(R)$ are $[0, 1]$-valued. If we denote

$$W_a = -2\log\left(1 - \sqrt{\frac{2e}{d}}\psi_d(R)\right) \quad \text{and} \quad W_b := -\log(1 - R),$$

then it suffices to prove that $\mathbb{E}[W_a^2] < \infty$ and $\mathbb{E}[W_b^2] < \infty$.

$$\mathbb{E}[W_b^2] = \int_0^1 f_b(s)\,\mathrm{d}s \qquad \text{with } f_b(s) = \frac{(\log(1-s))^2}{s\Gamma(d/2)}\big(s\log\big(s^{-d/2}\big)\big)^{d/2}.$$

Let us observe that $f_b(s)$ tends to 0 as $s \to 0$ and in a neighborhood of 1, $f_b(s) \sim C_1(1-s)^{d/2}(\log(1-s))^2$ where $C_1 > 0$ is a constant. We deduce that f_b is integrable on the whole interval $[0, 1]$ which implies that $\mathbb{E}[W_b^2] < \infty$. For W_a we get $\mathbb{E}[W_a^2] = \int_0^1 f_a(s)\,\mathrm{d}s$ with

$$f_a(s) = \frac{4\log^2(1 - \sqrt{\frac{2e}{d}s\log(s^{-d/2})})}{s\Gamma(d/2)}\big(s\log\big(s^{-d/2}\big)\big)^{d/2}.$$

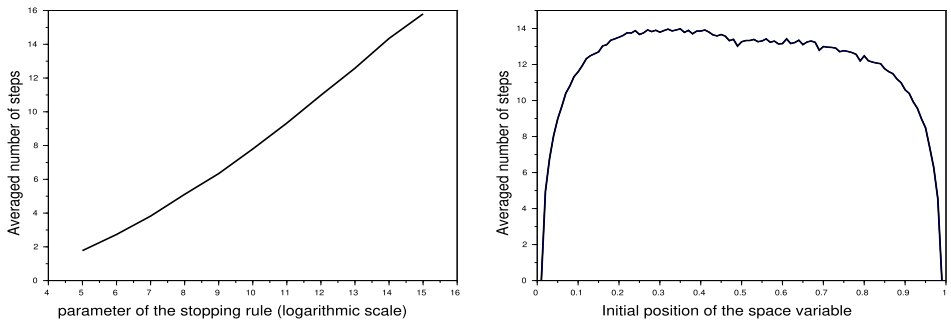

FIG. 12. *Averaged number of steps versus n for $\varepsilon = 0.5^n$ and $x = (0.5, 0, 0)$ (left), averaged number of steps versus u for $x = (u, 0, 0)$ and $\varepsilon = 0.0001$. In both situations*: 10,000 *trials*, $d = 3$, $t = 1$.

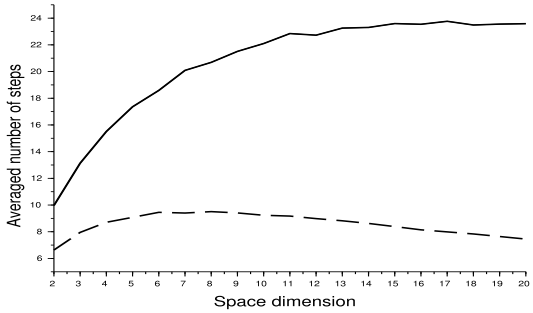

FIG. 13. *Averaged number of steps versus the dimension d for* $\varepsilon = 0.001$ (*dashed line*) *and* $\varepsilon = 0.0001$ (*solid line*). *In both situations*: 10,000 *trials*, $t = 1$ *and* $x = (0.5, 0, 0)$.

In a neighborhood of 0, we have $f_a(s) \sim C_2 s^{d/2} (\log s)^{d/2+1}$, in a neighborhood of 1, we observe $f_a(s) \sim C_3 (1-s)^{d/2+1}$ and finally in a neighborhood of $1/e$, $f_a(s) \sim C_4 \log^2 |s - \frac{1}{e}|$. We deduce that f_a is integrable on the whole interval $[0, 1]$ and $\mathbb{E}[W_a^2] < \infty$. $\square$

APPENDIX B: IMPROVEMENTS FOR THE CLASSICAL RANDOM WALK ON SPHERES

In this section, we focus our attention on the classical random walk on spheres. We consider an 0-thick domain $\mathcal{D}$, see the definition developed in (4.3), and the Euclidean distance to the boundary $d(x) = \delta(x, \partial\mathcal{D})$. The random walk is then defined as follows:

- We start with an initial condition X_0 and fix two parameters $\varepsilon > 0$ and $\beta \in]0, 1[$.
- While $d(X_n) > \varepsilon$, we construct

$$X_{n+1} = X_n + \beta d(X_n) \gamma_n, \tag{B.1}$$

where (γ_n) stands for a sequence of independent random variables uniformly distributed on the unit sphere in $\mathbb{R}^d$.

We adapt here several results of [2] to our particular situation. Let us recall that U is the *energy function* defined by (4.10) which is based on the set of measures $\mathcal{M}$, defined by (4.5), and on the Riesz potential. Since $\mathcal{D}$ is a 0-thick domain, the following lemma holds.

LEMMA B.1. *There exist two constants* $\delta > 0$ *and* $\eta > 0$, *such that*: *for any* $y \in \mathcal{D}$ (*we define* x *the closest point of* y *belonging to the boundary*) *and any measure* $\mu \in \mathcal{M}$, *we have*:

1. *either* $U(z) > U^{\mu}(z) + 1$ *whenever* $\|z - x\| < \delta d(y)$ *and* $d(z) > \delta/4\, d(y)$,
2. *or* $\mu(B(y, 2d(y))) \geq \eta d(y)^d$.

This lemma, which is quite general and is not directly linked to the random walk, has an important consequence on it (for the proof of Lemma B.1, see [2]).

PROPOSITION B.2. *Let us consider δ the constant of Lemma B.1 and the random walk $(X_n)_{n\geq 0}$ defined by (B.1) with $\beta \in]1-\delta/2, 1-\delta/4[$. Then there exists a constant $L>0$ such that the sequence $U_n := U(X_n)$ satisfies*

$$\mathbb{E}[U_{n+1} - U_n | U_n] > L \qquad \forall n \geq 0.$$

In [2], the authors consider a general random walk defined by (B.1). They prove that there exist an integer k and a constant $L>0$ such that $\mathbb{E}[U_{n+k} - U_n|U_n] > L$. Here, we adapt the proof by introducing a particular condition on the parameter β which permits in fact to set $k=1$.

PROOF OF PROPOSITION B.2. Let us consider X_n. Due to the weak compactness of the set of measures $\mathcal{M}$ (see Remark 4.3), there exists a measure $\mu \in \mathcal{M}$ such that

$$U_n = U(X_n) = U^{\mu}(X_n).$$

For this particular measure, either the first or the second point of the previous lemma are satisfied.

Step 1. Let us assume that the first point is satisfied, that is, $U(z) > U^{\mu}(z) + 1$ when $\|z-x\| < \delta d(y)$ and $d(z) > \delta/4\, d(y)$. Since $U^{\mu}(X_n)$ is a submartingale, we get

$$\begin{aligned}\mathbb{E}[U_{n+1} - U_n|X_n] &= \mathbb{E}\big[U_{n+1} - U^{\mu}_{n+1}|X_n\big] + \mathbb{E}\big[U^{\mu}_{n+1} - U^{\mu}_n|X_n\big] \\ &\geq \mathbb{E}\big[U_{n+1} - U^{\mu}_{n+1}|X_n\big] \\ &\geq \mathbb{P}\big(\|X_{n+1} - x_n\| < \delta d(X_n),\, d(X_{n+1}) > (\delta/4) d(X_n)|X_n\big),\end{aligned}$$

where x_n is the closest point of X_n on the boundary $\partial\mathcal{D}$. We denote by $u_n = \frac{x_n - X_n}{d(X_n)}$ which belongs to the unit sphere. Using the definition of the random walk and the particular choice of the parameter β, we get immediately

$$d(X_{n+1}) > (1-\beta) d(X_n) > \delta/4 d(X_n),$$

and

$$\begin{aligned}\|X_{n+1} - x_n\| &= d(X_n)\|u_n - \beta\gamma_n\| \leq d(X_n)\big((1-\beta)\|\gamma_n\| + \|\gamma_n - u_n\|\big) \\ &= d(X_n)\big(1 - \beta + \|\gamma_n - u_n\|\big) < d(X_n)\big(\delta/2 + \|\gamma_n - u_n\|\big).\end{aligned} \tag{B.2}$$

Let us recall that u_n is a unit vector. Then we define the set Γ_{u_n} of points u belonging to the unit sphere of dimension d such that $\|u - u_n\| < \delta/2$. Let us just note that Γ_{u_n} is a nonempty open set.

We observe that $\mathbb{P}(\gamma_n \in \Gamma_{u_n}) =: p > 0$ for any $n \geq 0$ and does not depend on u_n due to rotational invariant of the distribution. Furthermore, for any $\gamma_n \in \Gamma_{u_n}$, (B.2) implies that $\|X_{n+1} - x_n\| < \delta d(X_n)$. Therefore,

$$\begin{aligned}\mathbb{E}[U_{n+1} - U_n | X_n] &\geq \mathbb{P}\big(\|X_{n+1} - x_n\| < \delta d(X_n),\, d(X_{n+1}) > (\delta/4) d(X_n) | X_n\big) \\ &\geq \mathbb{P}(\gamma_n \in \Gamma_{u_n}) = p > 0.\end{aligned}$$

Step 2. The second case concerns the condition

$$\mu\big(B\big(y, 2d(y)\big)\big) \geq \eta d(y)^d.$$

By the Green formula, for a $\mathcal{C}^2$-smooth function h,

$$\begin{aligned}\mathbb{E}\big[h(X_{n+1}) | X_n\big] - h(X_n) &= \int_{\mathbb{S}(X_n, \beta d(X_n))} h(y)\, \mathrm{d}\sigma(y) - h(X_n) \\ &= \int_0^{\beta d(X_n)} r^{1-d} \int_{B(X_t, r)} \Delta h(y)\, \mathrm{d}V(y)\, \mathrm{d}r.\end{aligned}$$

Since $\Delta U^\mu(y) = 2(d+2) \int_0^\infty \frac{\mu(B(y,r))}{r^{d+3}}\, \mathrm{d}r$ outside the support of the measure μ (consequently U^μ is a $\mathcal{C}^2$-function in the domain $\mathcal{D}$), then, for any y satisfying $\|y - X_n\| \leq \beta d(X_n)$, we get

$$\begin{aligned}\Delta U^\mu(y) &\geq 2(d+2)\mu\big(B\big(X_n, 2d(X_n)\big)\big) \int_{(2+\beta)d(X_n)}^\infty \frac{\mathrm{d}r}{r^{d+3}} = \frac{2\mu(B(X_n, 2d(X_n)))}{((2+\beta)d(X_n))^{d+2}} \\ &\geq \frac{2\eta}{(2+\beta)^{d+2}}\, d(X_n)^{-2}.\end{aligned}$$

Applying the previous results to the particular smooth function $h = U^\mu$, we deduce:

$$\begin{aligned}\mathbb{E}[U_{n+1} - U_n | X_n] &= \mathbb{E}\big[U^\mu(X_{n+1}) | X_n\big] - U^\mu(X_n) \\ &\geq C d(X_n)^{-2} \int_0^{\beta d(X_n)} r\, \mathrm{d}r = \frac{C\beta^2}{2}\end{aligned}$$

for some positive constant C depending on η, β and d.

Since $\mathbb{E}[U_{n+1} - U_n | U_n] = \mathbb{E}[U_{n+1} - U_n | X_n]$, we obtain the announced result. □

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