

Analysis and Comparison of Green's Function First-Passage Algorithms with “Walk on Spheres” Algorithms

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Abstract

We analyze the optimization of the running times of Green's function first-passage (GFFP) algorithms. The running times for these new first-passage (FP) algorithms [1–4], which use exact Green's functions for the Laplacian to eliminate the absorption layer in the “walk on spheres” (WOS) method [5–9], are compared with those for WOS algorithms. It has been empirically observed that GFFP algorithms are more efficient than WOS algorithms when high accuracy is required [2–4]. Additionally, it has been observed that there is always an optimal distance from the surface of the absorbing boundary, δ_I , for a GFFP algorithm within which a FP surface can be permitted to intersect the boundary [2–4]. In this paper, we will provide a rigorous complexity analysis consistent with these observations. This analysis is based on estimating the numbers of WOS and GFFP steps needed for absorption on the boundary, and the complexity and running times of each WOS and GFFP step. As an illustration, we analyze the running times for calculating the capacitance of the unit cube using both GFFP and WOS.

Key words: Green's function first-passage (GFFP), “walk on spheres” (WOS), complexity analysis

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1 Introduction

It is well known that random walk methods or Monte Carlo diffusion algorithms can be used to solve parabolic and elliptic partial differential equa-

tions [5,10–14]. The probability of finding an isotropic and spatially homogeneous random walker at a given point in space-time satisfies the diffusion equation. The steady state first-passage distribution of a random walker can also be used to solve the Laplace equation.

The diffusive motion of the random walker can be simulated on discrete grids or in continuum space. In continuum space, the motion of the free Brownian particles (random walkers) can be realized using a first-passage (FP) probability distribution [5,12,15,16] to enable large steps to be taken. The FP probability, $w(\mathbf{x}; \mathbf{x}_0)$, is the probability of hitting the vicinity of \mathbf{x} on the bounding surface (FP surface) for the first time with a Brownian particle starting at \mathbf{x}_0 inside the bounding surface. If the bounding surface is a sphere and a Brownian particle starts from the center of the sphere, the FP probability distribution yields the hitting probability distribution on the bounding surface where the Brownian particle, starting from the center of the sphere, reaches the surface of the sphere for the first time. This hitting probability is uniform over the spherical surface for isotropic Brownian motion. Instead of following the complicated zig-zag motions of a nondifferentiable Brownian trajectory, the FP probability distribution allows us to move Brownian particles from one FP surface to the next by constructing new FP geometries at each step. The particular diffusion Monte Carlo method that uses only the FP probability distribution of a sphere is called the "walk on spheres" (WOS) method [5–9]. As we will see below, there are more general versions of these FP methods.

Simulation of diffusion in continuum space is more accurate than that on spatially discretized grids because it avoids the error which is introduced with a discrete grid [17]. However, if only the simplest FP distribution (spherical FP surface) is used, like in the WOS method, another error is introduced. This is due to the fact that with spherical FP surfaces, no walker ever terminates its walk on an arbitrary boundary due to geometric considerations. Thus we are required to add an absorption layer in WOS to provide a geometrical circumstance when absorption on the boundary can occur [15] (see Fig. 1). The absorption layer, which we call the δ_h -layer in this paper, is the region near the surface of the given boundary within which a Brownian particle is declared to be absorbed on the boundary.¹ A Brownian particle is considered to be absorbed on the absorbing boundary if it lies a small distance (inside the absorbing layer), δ_h , from the absorbing boundary.

The need for an absorbing boundary was removed by using the set of Laplacian surface Green's functions given by Given, Hubbard, and Douglas [1]. They allowed the classical WOS FP surface to intersect the absorbing boundary (see

¹ In this paper we refer to the δ_h -layer and use δ_h itself to refer to the thickness of this layer.

Fig. 2): this introduces a new family of possible FP surfaces. These FP surfaces consist of the intersected boundary surface and the spherical FP surface outside of the boundary. If the FP surface is sufficiently simple, geometrically, to construct a surface Green's function for the Laplacian inside the bounding surface, this surface Green's function can be used as the FP probability to construct absorbed Brownian trajectories.

A set of such Laplacian surface Green's functions was obtained based on FP probabilistic potential theory [10,11]. The probability density, $\sigma_1(\mathbf{x}_1)$, at point \mathbf{x}_1 of a Brownian particle starting from point \mathbf{x}_0 and being absorbed at point \mathbf{x}_1 is given by

$$\sigma_1(\mathbf{x}_1) = \frac{\partial}{\partial \mathbf{n}} G(\mathbf{x}_0, \mathbf{x}_1), \quad (1)$$

where \mathbf{n} is the inward-pointing unit normal vector to the absorbing surface at \mathbf{x}_1 and $G(\mathbf{x}_0, \mathbf{x}_1)$ is the Green's function for the Laplacian with unit source at the point \mathbf{x}_0 and a homogeneous Dirichlet boundary condition. Using the known Green's functions for the electrostatic problem of two conducting intersecting spheres, and the method of inversion for other geometries, Given, Hubbard, and Douglas [1] tabulated the necessary FP probability density functions to exactly deal with absorbing boundaries that are either flat or spherical. This enhancement to WOS was called the Green's function first-passage (GFFP) algorithm [1–4]. Using GFFP leaves only the statistical sampling error in this Monte Carlo diffusion method.

Two properties that have been observed in numerical calculations are that GFFP algorithms are more efficient than WOS algorithms when enough accuracy is required, and for a GFFP algorithm there is always an optimal choice for δ_I , the distance from the surface of the absorbing boundary within which a FP surface can intersect the boundary [1–3]. In this paper, we analyze the optimization of GFFP algorithms with respect to δ_I , and compare the running times of GFFP algorithms with those of WOS algorithms. This analysis is based on a comparison of the number of WOS and GFFP steps needed for absorption on the boundary, and the running times of each WOS and GFFP step. Using this complexity analysis, we provide a theoretical basis for the observation that GFFP algorithms are more efficient than WOS algorithms when enough accuracy is required. Also, we demonstrate the theoretical reason for the existence of an optimal δ_I for the GFFP algorithm. As an example, numerical experiments are presented for the calculation of the capacitance of the unit cube, a notoriously difficult problem.

This paper is organized as follows. In § II, we analyze the running times of GFFP and WOS algorithms and illustrate the validity of our analysis with the unit cube capacitance calculation. In § III we summarize our results and

provide concluding remarks.

2 Analysis of GFFP and WOS algorithms

In this section, we analyze the running times of GFFP and WOS algorithms and show that GFFP algorithms are more efficient than WOS when enough accuracy is required. Also, we demonstrate the theoretical reason for the existence of an optimal δ_I for the GFFP algorithm, which minimizes the running time. As an illustration, we empirically analyze the calculation of the unit cube capacitance using both WOS and GFFP algorithms.

WOS algorithms use the uniform FP probability on a spherical FP surface to simulate rapid Brownian trajectories in free diffusion region with a δ_h -layer for capture and termination on the absorbing boundary [12] (see Fig. 1). GFFP algorithms are refinements of these WOS algorithms that remove the δ_h -layer using a set of Laplacian Green's functions to provide exact terminal FP probabilities. This set of Laplacian Green's functions allows us to intersect the absorbing boundary giving the FP probability distribution for the non-trivial FP surface [1]. The FP surface consists of the intersected boundary surface and the spherical FP surface outside the boundary (see Fig. 2). However in practice and for efficiency, another layer, called the δ_I -layer, is introduced such that we use WOS outside the δ_I -layer and GFFP inside the δ_I -layer.² Note that a δ_h -layer can be used when WOS is used outside a δ_I -layer. This entails a finite probability of terminating Brownian trajectories when WOS is used outside the δ_I -layer (see Fig. 2).

The average number of steps required for a Brownian particle to be absorbed in a δ_h -layer for the WOS algorithm is $O(|\ln \delta_h|)$ [12]. This means that the total running time of a WOS algorithm is proportional to $|\ln \delta_h|$, and as δ_h goes to zero the running time goes to infinity. Fig. 3 shows the average number of steps required for a Brownian particle to be absorbed in the δ_h -layer for the WOS calculation of the unit cube capacitance. This figure confirms the theory just cited. In GFFP algorithms, the average number of steps required for a Brownian particle to be absorbed on the boundary is expected to be monotonically increasing with respect to δ_I . This means that as δ_I goes to zero the average number of steps will go to zero because the probability of being absorbed will go to one as the Brownian particle approaches the boundary. In Fig. 4, it is shown that in the GFFP algorithm for cube capacitance, the average number of steps required for a Brownian particle to be absorbed on the boundary is monotonically increasing in δ_I .

² Again, we refer to both the layer and its width with δ_I .

The running times for WOS and GFFP algorithms, T_w and T_g respectively, can be expressed as

$$\begin{aligned} T_w &= O(N_w t_w) \\ &= O(|\ln \delta_h| t_w), \end{aligned} \tag{2}$$

$$\begin{aligned} T_g &= O(N'_w t_w + N_g t_g) \\ &= O(t_w [(1 + q + q^2 + q^3 + \dots) |\ln \delta_I|] + N_g t_g) \\ &= O\left(t_w \left(\frac{1}{1-q}\right) |\ln \delta_I| + N_g t_g\right) \\ &= O\left(t_w \left(\frac{1}{p}\right) |\ln \delta_I| + N_g t_g\right) \\ &= O(|\ln \delta_I| t_w + \alpha t_w f(\delta_I)), \end{aligned} \tag{3}$$

where N_w and N'_w are the average numbers of WOS steps for the WOS algorithm and GFFP algorithm respectively, and t_w , the CPU cost per WOS step. Also, N_g is the average number of GFFP steps required, and t_g is the CPU cost per GFFP step. In addition, we define p to be the probability of terminating the Brownian walk within δ_I -layer during a GFFP algorithm. This means that $q = (1 - p)$ is the probability of escaping a δ_I -layer without absorption after initially entering a δ_I -layer. Usually $0 \ll p < 1$ for a finite small δ_I . Moreover, $f(\delta_I)$, the average number of GFFP steps, is assumed to be a monotonically increasing positive function. This assumption comes from observing many previous numerical calculations [2–4]. It should be noted that as δ_I goes to zero, p goes to one and that q^j represents the probability of j consecutive failures of terminating the same walk. In practice, j is less than 10 but it is convenient to consider an infinite number of failures, which can be bounded by the geometric series $\sum_{j=1}^{\infty} q^j < 1/p$. Also, we introduce a positive constant, $\alpha > 1$, such that $t_g = \alpha t_w$ since the cost of each WOS step is less than a GFFP step.

In GFFP algorithms (see Fig. 2), WOS is used outside the δ_I -layer for efficiency (the first term in Eq. 3) and GFFP inside δ_I -layer (the second term in Eq. 3), because the cost per WOS step is much smaller than a GFFP step. There are two ways of using WOS in GFFP algorithms: with or without the δ_h -layer (see Fig. 2). In GFFP algorithms, there is a finite probability of being absorbed in the δ_h -layer when WOS with the δ_h -layer is used when the Brownian particle is outside the δ_I -layer. In this case, assuming that the finite probability of being absorbed in the δ_h -layer is linear in δ_h when δ_h is small, we can add $-k\delta_h$ to Eq. 3 with k being a positive constant.

From the running times, it can be noted that for a finite δ_I there exists a δ_h

such that the running time of a GFFP algorithm is always less than that of WOS:

$$O(|\ln \delta_h|) - O(|\ln \delta_I|) > \alpha f(\delta_I). \quad (4)$$

Recall that $|\ln \delta_h|$ goes to infinity as δ_h goes to zero. Also for T_g it can be readily shown from the last equation of Eq. 3 that for every positive α and γ there exists an optimal choice for δ_I assuming that $f(\delta_I)$ obeys a power law, $f(\delta_I) = \delta_I^\gamma$:

$$\delta_I = \left(\frac{1}{\alpha\gamma} \right)^{1/\gamma}. \quad (5)$$

This assumption of a power law comes from many observations of previous numerical calculations [2–4] (see Fig. 4). Even though the CPU time of a GFFP step is greater than that of a WOS step, there is an optimal distance for δ_I for which the overall running time of a GFFP algorithm is smaller than that of the corresponding WOS algorithm!

Fig. 5 shows the overall running times required to calculate the capacitance of the unit cube, to a fixed tolerance, using the GFFP algorithm. The figure shows that, for each value of δ_h , there is a non-zero optimal value for δ_I . In this example, δ_I is about 0.035, γ about 0.3 and α about 9. Also, this figure suggests that WOS with a δ_h -layer outside the δ_I -layer and GFFP inside the δ_I -layer is better than just using WOS without the δ_h -layer outside the δ_I -layer and GFFP inside the δ_I -layer if we can control the error from the absorbing boundary layer. There is a finite probability of being absorbed in the δ_h -layer when WOS with a δ_h -layer is used outside the δ_I -layer. This error from the δ_h -layer, in general, can always be made smaller than the statistical sampling error [9,18]. A technique for empirically estimating this δ_h -layer error uses a single Brownian trajectory to both estimate the δ_h and the $\delta_h/10$ error. The difference between these two correlated estimates gives a measure of the δ_h behavior of the error due to the finite width of the δ_h -layer. By adjusting δ_h , one can make this error less than that arising from the statistical sampling error. Thus if one increases the number of Brownian trajectories in order to decrease the statistical error, one must also reduce δ_h in order to reduce the δ_h -layer error to be less than the statistical sampling error. Another way is to use the error analysis in [19]. The δ_h -layer error is linear in δ_h for small δ_h so that we can make this error smaller than the statistical error. However, in this case we need to perform the δ_h -error analysis prior to applying GFFP algorithms.

In our current GFFP algorithms, there are only two intersecting geometries in relation to optimization: a sphere that intersects a flat absorbing boundary

and a sphere that intersects an absorbing spherical boundary. Here, there are two geometric parameters in both intersecting geometries: δ_I and the radius of the intersecting sphere. However, in regard to optimization there is only one geometric parameter, δ_I . For a fixed δ_I , the radius of the intersecting sphere should be as large as possible because it will increase the probability of being absorbed on the boundary. Therefore, in the case of the unit cube capacitance calculation, the radius of the intersecting sphere is taken as the distance to the nearest cube edge.

For different geometries, the optimal choices will be different as the numbers of WOS and GFFP steps depend on the geometry [3]. So, for each GFFP algorithm we could and should find the corresponding optimal value.

3 Summary and Conclusions

This paper analyzes the running times of GFFP and WOS algorithms and shows that GFFP algorithms are more efficient than WOS when enough accuracy is required. Even though running time cost per GFFP step is greater than time cost per WOS step, the average number of WOS steps required for a Brownian trajectory to be absorbed in the δ_h -layer is $O(|\ln \delta_h|)$, so that as δ_h goes to zero the running time of WOS algorithms goes to infinity. Also, it is shown that in any GFFP algorithm there is always an optimal choice for δ_I , the distance from the surface of the absorbing boundary within which a FP surface can intersect the boundary. These analyses are illustrated within the calculation of capacitance of the unit cube. The existence of the optimal choice for δ_I for the calculation of the unit cube capacitance was mentioned in the paper of Given *et al.* [1].

The optimal choice for δ_I depends on the particular application because the numbers of WOS and GFFP steps depend on the geometry. So, for each GFFP algorithm we could and should find the corresponding optimal value.

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References

- [1] J. A. Given, J. B. Hubbard, and J. F. Douglas. A first-passage algorithm for the hydrodynamic friction and diffusion-limited reaction rate of macromolecules. *J. Chem. Phys.*, 106(9):3721–3771, 1997.
- [2] C.-O. Hwang, J. A. Given, and M. Mascagni. On the rapid calculation of permeability for porous media using Brownian motion paths. *Phys. Fluids A*, 12(7):1699–1709, 2000.
- [3] C.-O. Hwang, J. A. Given, and M. Mascagni. The simulation-tabulation method for classical diffusion Monte Carlo. *J. Comput. Phys.*, 174(2):925–946, 2001.
- [4] C.-O. Hwang, J. A. Given, and M. Mascagni. Rapid diffusion Monte Carlo algorithms for fluid dynamic permeability. *Monte Carlo Methods and Applications*, 7(3-4):213–222, 2001.
- [5] M. E. Müller. Some continuous Monte Carlo methods for the Dirichlet problem. *Ann. Math. Stat.*, 27:569–589, 1956.
- [6] A. Haji-Sheikh and E. M. Sparrow. The solution of heat conduction problems by probability methods. *Journal of Heat Transfer*, 89:121–131, 1967.
- [7] H.-X. Zhou, A. Szabo, J. F. Douglas, and J. B. Hubbard. A Brownian dynamics algorithm for calculating the hydrodynamic friction and the electrostatic capacitance of an arbitrarily shaped object. *J. Chem. Phys.*, 100(5):3821–3826, 1994.
- [8] I. C. Kim and S. Torquato. Effective conductivity of suspensions of overlapping spheres. *J. Appl. Phys.*, 71(6):2727–2735, 1992.
- [9] T. E. Booth. Exact Monte Carlo solution of elliptic partial differential equations. *J. Comput. Phys.*, 39:396–404, 1981.
- [10] S. C. Port and C. J. Stone. *Brownian Motion and Classical Potential Theory*. Academic Press, New York, 1978.
- [11] M. Freidlin. *Functional Integration and Partial Differential Equations*. Princeton University Press, Princeton, New Jersey, 1985.
- [12] K. K. Sabelfeld. *Monte Carlo Methods in Boundary Value Problems*. Springer-Verlag, Berlin, 1991.
- [13] K. K. Sabelfeld. Integral and probabilistic representations for systems of elliptic equations. *Mathematical and Computer Modelling*, 23:111–129, 1996.
- [14] R. Ettelaie. Solutions of the linearized Poisson-Boltzmann equation through the use of random walk simulation method. *J. Chem. Phys.*, 103(9):3657–3667, 1995.
- [15] L. H. Zheng and Y. C. Chiew. Computer simulation of diffusion-controlled reactions in dispersions of spherical sinks. *J. Chem. Phys.*, 90(1):322–327, 1989.

- [16] S. Torquato and I. C. Kim. Cross-property relations for momentum and diffusional transport in porous media. *J. Appl. Phys.*, 72(2):2612–2619, 1992.
- [17] S. B. Lee, I. C. Kim, C. A. Miller, and S. Torquato. Random-walk simulation of diffusion-controlled processes among static traps. *Phys. Rev. B*, 39:11833–11839, 1989.
- [18] T. E. Booth. Regional Monte Carlo solution of elliptic partial differential equations. *J. Comput. Phys.*, 47:281–290, 1982.
- [19] M. Mascagni and C.-O. Hwang. ϵ -shell error analysis in “Walk On Spheres” algorithms. *Math. Comput. Simulat.*, submitted, 2001.

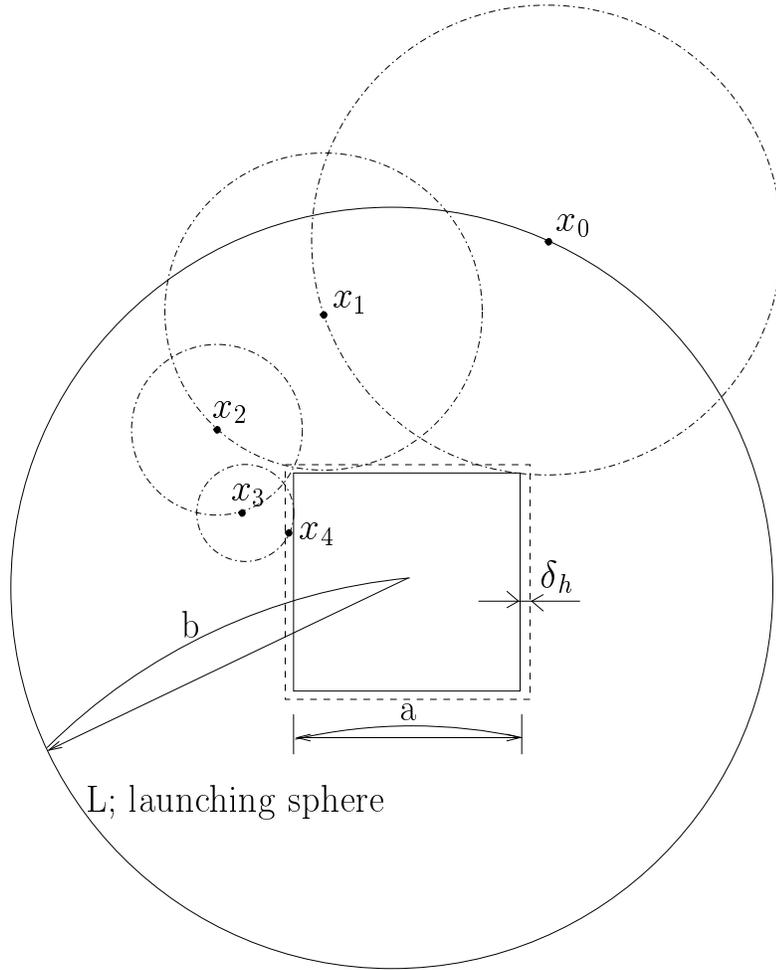


Fig. 1. A schematic side view that illustrates an absorbed series of FP jumps in WOS. In WOS, the boundary is thickened by δ_h , and when a Brownian particle is initiated with uniform probability from the launching sphere, L of radius b , and enters this δ_h -absorption layer the Brownian trajectory is terminated.

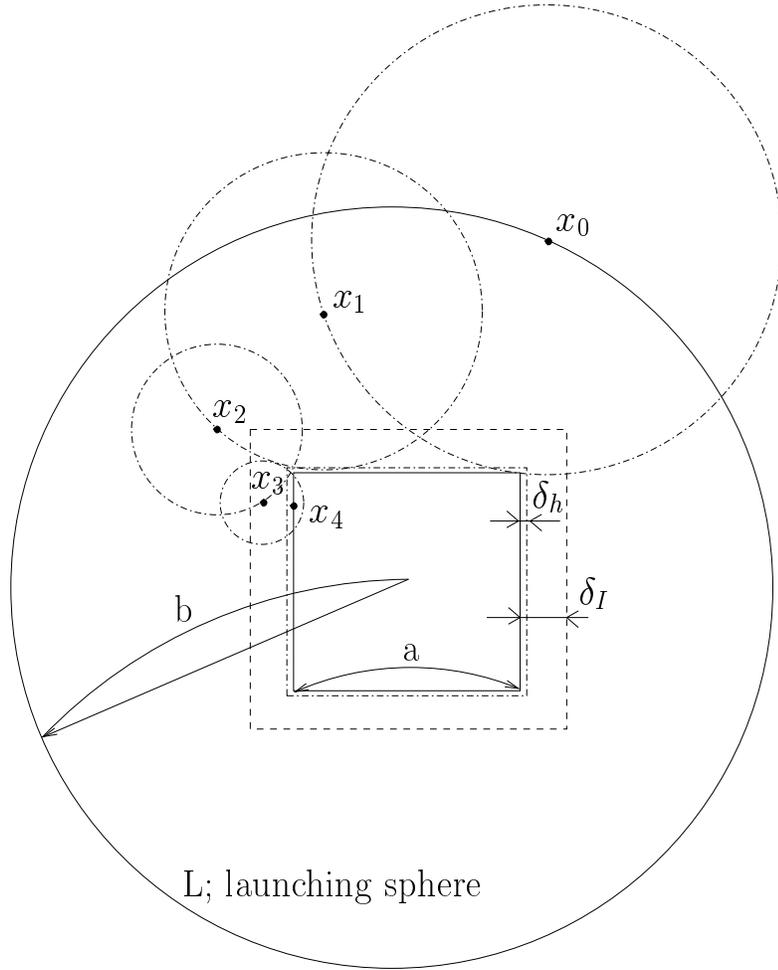


Fig. 2. A schematic side view that illustrates an absorbed series of FP jumps in GFFP with δ_h -layer. In this illustration, δ_I -boundary layer usage is shown; when a Brownian particle is initiated with uniform probability from the launching sphere, L of radius b , and reaches inside the δ_I -boundary layer, it begins to intersect the cube.

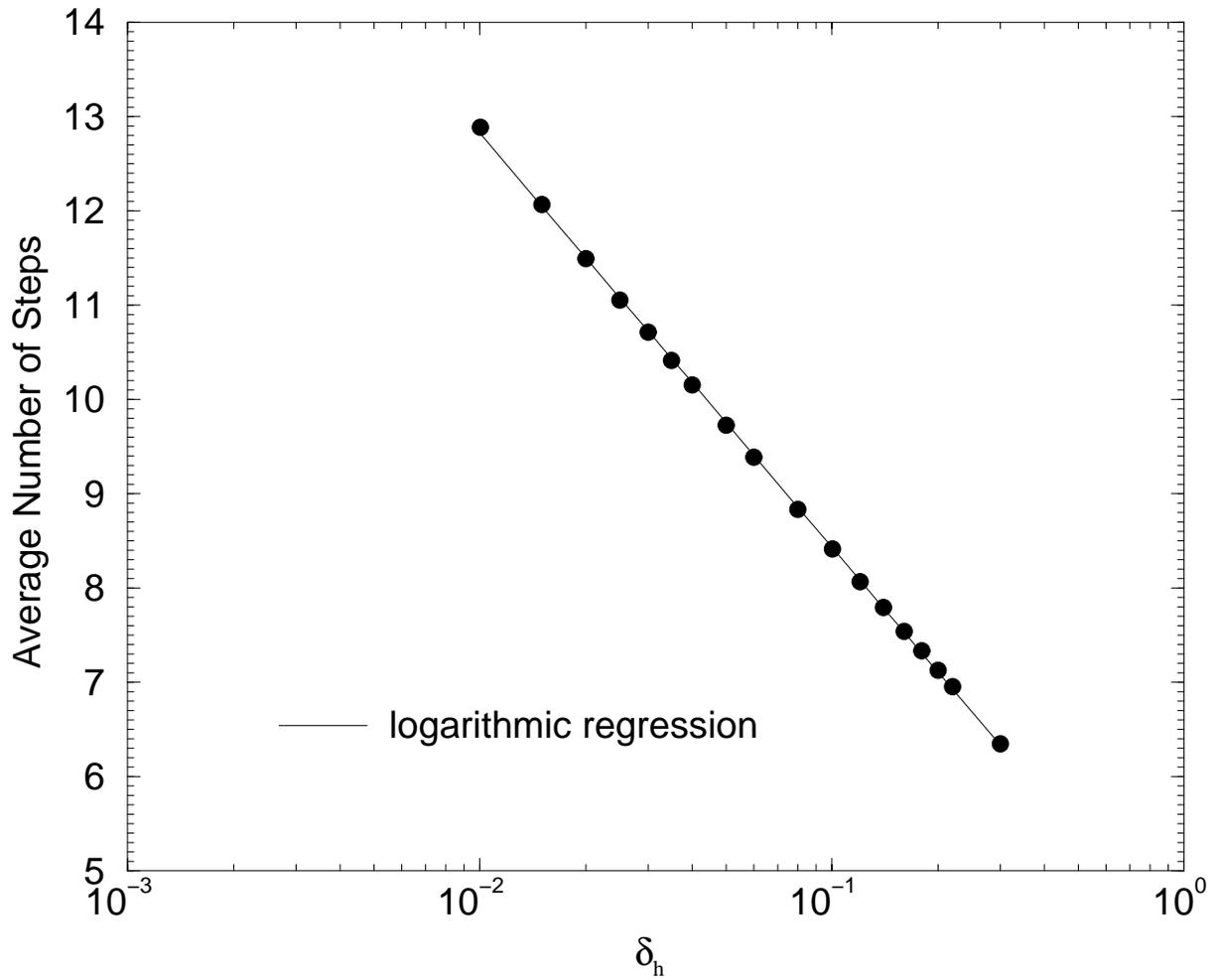


Fig. 3. Average number of steps for WOS on the calculation of the capacitance of the unit cube: δ_h is the absorption layer thickness and it shows the usual relation of the running time for WOS algorithms, $O(|\ln \delta_h|)$.

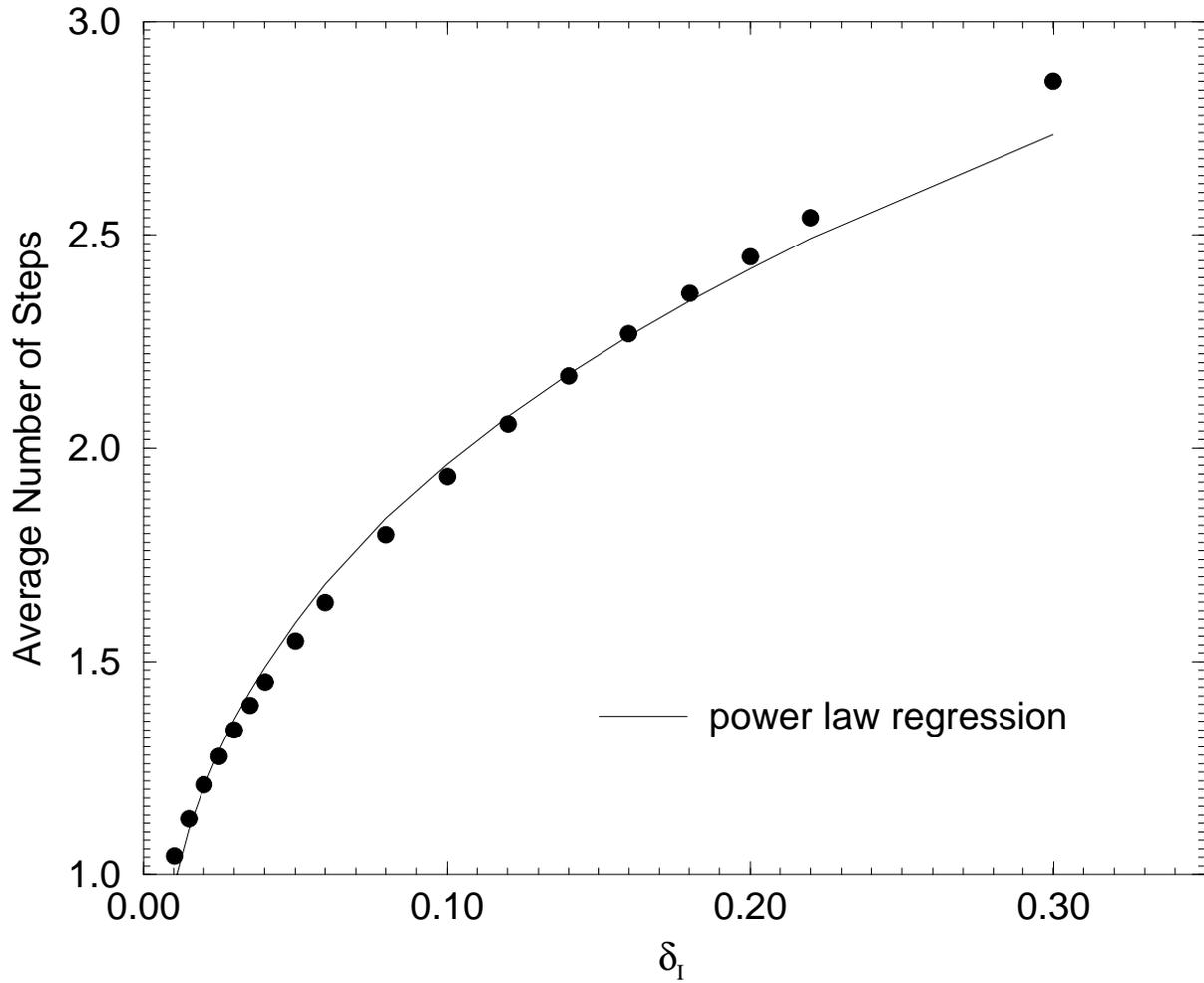


Fig. 4. Average number of steps for GFFP: δ_I is the distance within which the FP surface that intersects the surface of the cube can be used. The power law regression shows that the average number of steps is $O(\delta_I^{0.3})$.

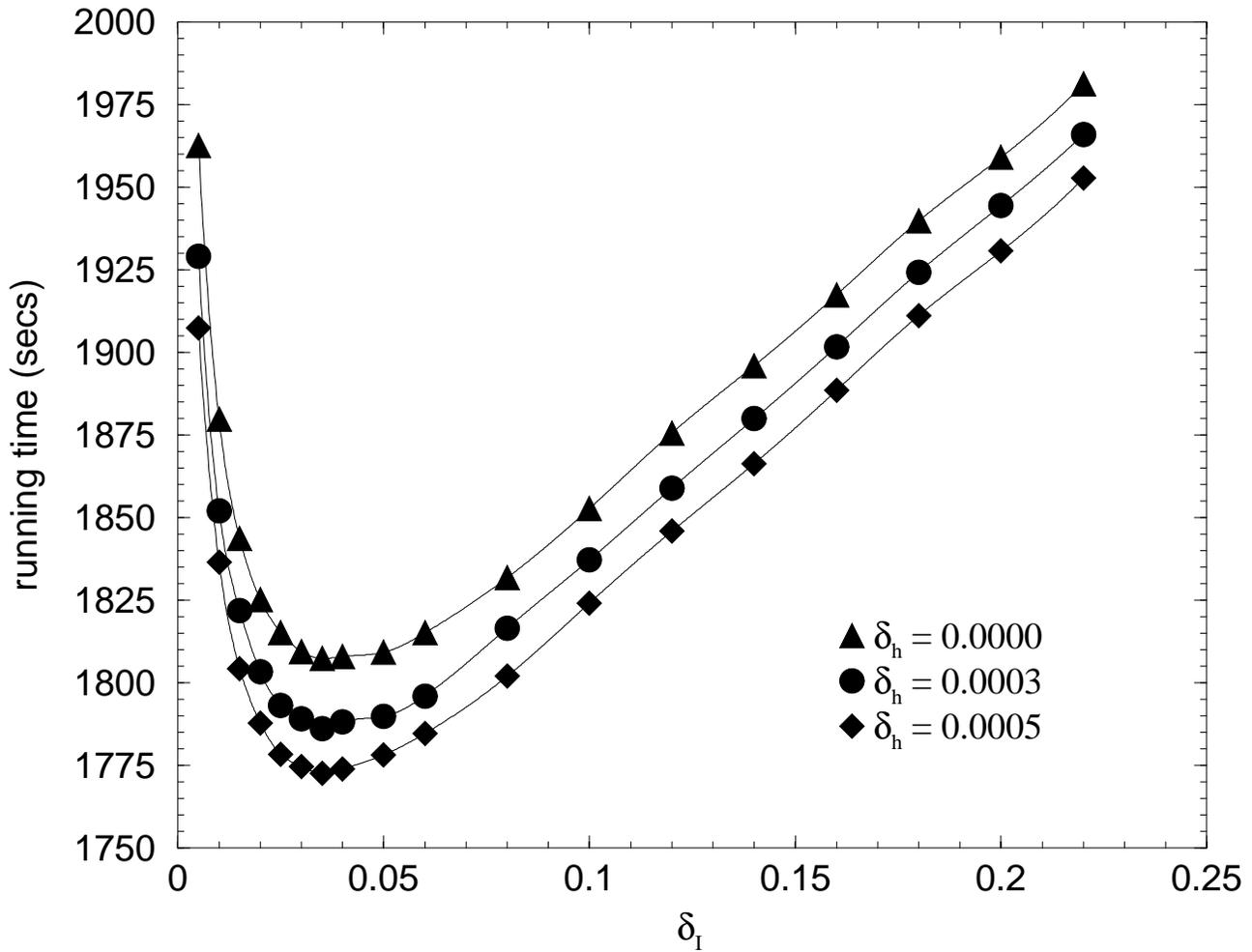


Fig. 5. Running times required to calculate the capacitance of the unit cube, to a fixed tolerance, using the GFFP method. The δ_h and δ_I are the distances from the surface of the cube within which a Brownian particle is declared, to be a "hit", i.e., an absorption event has occurred, and to use a FP surface that intersects the surface of the cube respectively. The figure shows that, for each value of δ_h , there is a non-zero optimal value for δ_I . The WOS method is given by $\delta_I = 0$.