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 [J. Chem. Phys. 106 (9) (1997) 3721; Phys. Fluids A 12 (7) (2000) 1699; J. Comput. Phys. 174 (2) (2001) 925; Monte Carlo Meth. Appl. 7 (3–4) (2001) 213], which use exact Green’s functions for the Laplacian to eliminate the absorption layer in the “Walk on Spheres” (WOS) method [Ann. Math. Stat. 27 (1956) 569; J. Heat Transfer 89 (1967) 121; J. Chem. Phys. 100 (5) (1994) 3821; J. Appl. Phys. 71 (6) (1992) 2727; J. Comput. Phys. 59 (1981) 396], 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 [Phys. Fluids A 12 (7) (2000) 1699; J. Comput. Phys. 174 (2) (2001) 925; Monte Carlo Meth. Appl. 7 (3–4) (2001) 213]. Additionally, it has been observed that there is always an optimal distance from the surface of the absorbing boundary, $\delta$, for a GFFP algorithm within which a FP surface can be permitted to intersect the boundary [Phys. Fluids A 12(7) (2000) 1699; J. Comput. Phys. 174 (2) (2001) 925; Monte Carlo Meth. Appl. 7 (3–4) (2001) 213]. 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.

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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 equations [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, \[ w(x, x_0), \]

is the probability of hitting the vicinity of \( x \) on the bounding surface (FP surface) for the first time with a Brownian particle starting at \( x_0 \) 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 \( \delta_h \)-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. A Brownian particle is considered to be absorbed on the absorbing boundary if it lies a small distance (inside the absorbing layer), \( \delta_h \), 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 et al. [1]. They allowed the classical WOS FP surface to intersect the absorbing boundary (see 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, \( \sigma_1(x_1) \), at point \( x_1 \) of a Brownian particle starting from point \( x_0 \) and being absorbed at point \( x_1 \) is given by

\[
\sigma_1(x_1) = \frac{\partial}{\partial n} G(x_0, x_1),
\]

1 In this paper, we refer to the \( \delta_h \)-layer and use \( \delta_h \) itself to refer to the thickness of this layer.
Fig. 1. A schematic side view that illustrates an absorbed series of FP jumps in WOS. In WOS, the boundary is thickened by $\delta_h$, and when a Brownian particle is initiated with uniform probability from the launching sphere, $L$, of radius $b$, and enters this $\delta_h$-absorption layer the Brownian trajectory is terminated.

Fig. 2. A schematic side view that illustrates an absorbed series of FP jumps in GFFP with $\delta_I$-layer. In this illustration, $\delta_I$-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 $\delta_I$-boundary layer, it begins to intersect the cube.
where $n$ is the inward-pointing unit normal vector to the absorbing surface at $x_1$ and $G(x_0, x_1)$ is the Green’s function for the Laplacian with unit source at the point $x_0$ 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 et al. [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 $\delta_I$, 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 $\delta_I$, 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 $\delta_I$ 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 Section 2, we analyze the running times of GFFP and WOS algorithms and illustrate the validity of our analysis with the unit cube capacitance calculation. In Section 3, 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 $\delta_I$ 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 $\delta_h$-layer for capture and termination on the absorbing boundary [12] (see Fig. 1). GFFP algorithms are refinements of these WOS algorithms that remove the $\delta_h$-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 $\delta_I$-layer, is introduced such that we use WOS outside the $\delta_I$-layer and GFFP inside the $\delta_I$-layer. Note that a $\delta_h$-layer can be used when WOS is used outside a $\delta_I$-layer. This entails a finite probability of terminating Brownian trajectories when WOS is used outside the $\delta_I$-layer (see Fig. 2).

The average number of steps required for a Brownian particle to be absorbed in a $\delta_h$-layer for the WOS algorithm is $O(|\ln \delta_h|)$ [12]. This means that the total running time of a WOS algorithm is proportional

$^2$ Again, we refer to both the layer and its width with $\delta_I$. 
to $\ln \delta_I$, and as $\delta_I$ 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 $\delta_I$-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 $\delta_I$. This means that as $\delta_I$ 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 $\delta_I$.

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

$$T_w = O(N_w t_w) = O(1/\ln \delta_h)$$

$$T_g = O(N'_w t_w + N_g t_g) = O((1 + q + q^2 + \cdots) \ln \delta_h) + N_g t_g$$

$$= O(t_w \left( \frac{1}{1-q} \right) \ln \delta_h) = O(t_w \left( \frac{1}{p} \right) \ln \delta_h)$$

$$= O(t_w \left( \frac{1}{1-q} \right) \ln \delta_h) + N_g t_g$$

where $N_w$ and $N'_w$ are the average numbers of WOS steps for the WOS algorithm and GFFP algorithm, respectively, and $t_w$ is 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 $\delta_I$-layer during a GFFP algorithm. This means that $q = (1-p)$ is the probability of escaping a $\delta_I$-layer without absorption after initially entering a $\delta_I$-layer. Usually $0 < q < 1$ for a finite small $\delta_I$. 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 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 \( \sum_{j=0}^{\infty} q^j \). Also, we introduce a positive constant, \( \alpha > 1 \), such that \( t_g \approx \alpha t_w \) since the cost of each WOS step is less than a GFFP step.

In GFFP algorithms (see Fig. 2), WOS is used outside the δI-layer for efficiency (the first term in Eq. (3) and GFFP inside δh-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 δh-layer (see Fig. 2). In GFFP algorithms, there is a finite probability of being absorbed in the δh-layer when WOS with the δh-layer is used when the Brownian particle is outside the δI-layer. In this case, assuming that the finite probability of being absorbed in the δh-layer is linear in δh when δh 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 δ1 there exists a δh such that the running time of a GFFP algorithm is always less than that of WOS:

\[
O(\ln \delta_1) - O(\ln \delta_h) > \alpha f(\delta_1). \tag{4}
\]

Recall that \( \ln \delta_h \) goes to infinity as δh goes to zero. Also for \( T_g \) it can be readily shown from the last equation of Eq. (3) that for every positive \( \alpha \) and \( \gamma \) there exists an optimal choice for \( \delta_1 \), assuming that \( f(\delta_1) \) obeys a power law, \( f(\delta_1) = \delta_1^{\gamma} \):

\[
\delta_1 = \left( \frac{1}{\alpha \gamma} \right)^{1/\gamma}. \tag{5}
\]
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 $\delta_I$ 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 method. The $\delta_h$ and $\delta_I$ 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 $\delta_h$, there is a non-zero optimal value for $\delta_I$. The WOS method is given by $\delta_I = 0$.

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Fig. 5 shows the overall running times required to calculate the capacitance of the unit cube, to a fixed tolerance, using the GFFP method. The figure shows that, for each value of $\delta_h$, there is a non-zero optimal value for $\delta_I$. In this example, $\delta_I$ is about 0.035, $\gamma$ about 0.3 and $\alpha$ about 9. Also, this figure suggests that WOS with a $\delta_h$-layer outside the $\delta_I$-layer and GFFP inside the $\delta_I$-layer is better than just using WOS without the $\delta_h$-layer outside the $\delta_I$-layer and GFFP inside the $\delta_I$-layer if we can control the error from the absorbing boundary layer. There is a finite probability of being absorbed in the $\delta_h$-layer when WOS with a $\delta_h$-layer is used outside the $\delta_I$-layer. This error from the $\delta_h$-layer, in general, can always be made smaller than the statistical sampling error [9,18]. A technique for empirically estimating this $\delta_h$-layer error uses a single Brownian trajectory to both estimate the $\delta_h$ and the $\delta_h/10$ error. The difference between these two correlated estimates gives a measure of the $\delta_h$ behavior of the error due to the finite width of the $\delta_h$-layer.

By adjusting $\delta_h$, 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 $\delta_h$ in order to reduce the $\delta_h$-layer error to be less than the statistical sampling error. Another way is to use the error analysis in [19]. The $\delta_h$-layer error is linear in $\delta_h$ for small $\delta_h$ so that we can make this error smaller than the statistical error. However, in this case we need to perform the $\delta_h$-layer 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: $\delta_I$ and the radius of the intersecting sphere. However, in regard to optimization there is only one geometric parameter, $\delta_I$. For a fixed $\delta_I$, 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 $\delta_h$-layer is $O(\ln \delta_h)$, so that as $\delta_h$ 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 $\delta_I$, the distance from the surface of the absorbing boundary within which a FP surface can intersect the boundary. The existence of the optimal choice for $\delta_I$ for the calculation of the unit cube capacitance was mentioned in the paper of Given et al. [1].

The optimal choice for $\delta_I$ 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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