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A new Green's function Monte Carlo algorithm for the estimation of the derivative of the solution of Helmholtz equation subject to Neumann and mixed boundary conditions

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ABSTRACT

The objective of this paper is the extension and application of a newly-developed Green's function Monte Carlo (GFMC) algorithm to the estimation of the derivative of the solution of the one-dimensional (1D) Helmholtz equation subject to Neumann and mixed boundary conditions problems. The traditional GFMC approach for the solution of partial differential equations subject to these boundary conditions involves "reflecting boundaries" resulting in relatively large computational times. My work, inspired by the work of K.K. Sabelfeld is philosophically different in that there is no requirement for reflection at these boundaries. The underlying feature of this algorithm is the elimination of the use of reflecting boundaries through the use of novel Green's functions that mimic the boundary conditions of the problem of interest. My past work has involved the application of this algorithm to the estimation of the solution of the 1D Laplace equation, the Helmholtz equation and the modified Helmholtz equation. In this work, this algorithm has been adapted to the estimation of the derivative of the solution which is a very important development. In the traditional approach involving reflection, to estimate the derivative at a certain number of points, one has to *a priori* estimate the solution at a larger number of points. In the case of a one-dimensional problem for instance, to obtain the derivative of the solution at a point, one has to obtain the solution at two points, one on each side of the point of interest. These points have to be close enough so that the validity of the first-order approximation for the derivative operator is justified and at the same time, the actual difference between the solutions at these two points has to be at least an order of magnitude higher than the statistical error in the estimation of the solution, thus requiring a significantly larger number of random-walks than that required for the estimation of the solution. In this new approach, identical amount of computational resources is needed irrespective of if we are trying to estimate the solution or the derivative. This becomes very significant in electromagnetic problems where the scalar/vector potential is the unknown in the PDE of interest, but the quantity of interest is the electric/magnetic field or in heat conduction problems where temperature of an object is the unknown variable in a PDE, but the quantity of interest is the spatial/temporal variation of the temperature. In this work, this algorithm is applied to the estimation of the derivative of the solution of the 1D Helmholtz equation which is the frequency domain version of both Maxwell's equations and the heat conduction equation. As a result the algorithm is an important first step in the development of computationally efficient GFMC algorithms for Neumann and mixed boundary condition problems. The numerical results have been validated by an exact,

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analytical solution and very good agreement has been observed. The long-term goal of this research is the application of this methodology to the numerical solution of the F region ionization problem in space plasma modeling.

1. Introduction

We begin our discussion with the exposition of the fundamentals behind the Green's function Monte Carlo (GFMC) solution [1] of differential equations. We consider a differential equation, with a differential operator L,

$$L\big[U(x)\big] = f(x), \tag{1}$$

where the solution $U(x)$ is a function of the one-dimensional position vector x defined in the region $a \le x \le b$. The function $f(x)$ is the forcing function. The Green's functions for Eq. (1) are the solutions of the differential equation

$$L\big[G(x|x_0)\big] = \delta(x - x_0), \tag{2}$$

subject to specified boundary conditions. We assume that the operator L is of the Sturm–Liouville [2] form:

$$L = \nabla \cdot \big[p(x)\nabla\big] + q(x), \tag{3}$$

where $p(x)$ and $q(x)$ are known functions of x. Using Green's integral representation [2], the solution at a point x_0 within the problem domain, $U(x)$ can be written as

$$U(x_0) = \int_a^b f(x_0)G(x|x_0)dx + \left[p(x)u(x)\frac{dG(x|x_0)}{dx}\right]_a^b - \left[p(x)G(x|x_0)\frac{dU(x)}{dx}\right]_a^b. \tag{4}$$

The first term on the right hand side of Eq. (4) represents the contribution from the forcing function. The second term represents the contribution of Dirichlet boundary conditions, while the third term represents the contribution of Neumann boundary conditions. In problems with inhomogeneous Dirichlet boundary conditions, homogeneous Dirichlet boundary conditions are imposed on the Green's function and the Green's integral representation from Eq. (4) reduces to

$$U(x_0) = \int_a^b f(x_0)G(x|x_0)dx_0 + \left[p(x)u(x)\frac{dG(x|x_0)}{dx}\right]_a^b. \tag{5}$$

In problems with inhomogeneous Dirichlet boundary conditions, the random-walker finds a reward in each one of two boundary points, where a walk is terminated. The termination of the random walk becomes a problem for Neumann and mixed boundary condition problems where the solution is not known at all points of the domain boundary. In Monte Carlo literature [3], these boundary conditions are formulated as partially "reflecting" as the random-walker is either absorbed in the problem boundary or is "reflected" back into the problem domain. I will now explain this problem of reflection within the context of the 1D Laplace equation.

2. Reflection at Neumann boundaries

Consider the equation

$$\frac{d^2U}{dx^2} = 0, \tag{6}$$

where U is the dependent variable of interest defined in the problem domain $0 \le x \le L$. The boundary conditions imposed on this problem are $U(0) = \alpha$ and $U(L) = \beta$. A traditional GFMC algorithm for this problem will be based on a Green's function given by

$$\frac{d^2G}{dx^2} = \delta(x - x_0), \tag{7}$$

defined on a problem domain $-h \le x \le h$, with homogeneous Dirichlet boundary conditions $G(-h|x_0) = 0$ and $G(+h|x_0) = 0$. The solution to Eq. (7) in a zero-centered notation (i.e., $x_0 = 0$) is given by

$$G(x|0) = \begin{Bmatrix} \frac{1}{2}(x-h), & x \ge 0 \\ -\frac{1}{2}(x+h), & x \le 0 \end{Bmatrix}. \tag{8}$$

Based on the 1D version of the Green's integral representation Eq. (5) along with homogeneous Dirichlet boundary conditions being imposed on the Green's function, the solution to Eq. (6) at the center of the one-dimensional problem domain can be written as

$$U(0) = \frac{1}{2}U(h) + \frac{1}{2}U(-h). \tag{9}$$

In a traditional GFMC algorithm, Eq. (9) is used to generate the random walks. The random walker either hops to the left or to the right with equal probability (without any restriction on the hop size) until it is absorbed at one of the boundaries. An estimate of the solution at any given point $x = x^*$ within the problem domain $0 \le x \le L$ is given by

$$U(x^*) = \frac{N_\alpha \alpha + N_\beta \beta}{N_\alpha + N_\beta}, \tag{10}$$

where the number of times the random walker hits the $x = 0$ and the $x = L$ boundary are N_α and N_β respectively. Now let us consider the solution of Eq. (6) defined on the problem domain $0 \le x \le L$, but with the boundary conditions $U(0) = \alpha$ and $\{dU/dx\}_{x=L} = \beta$. It is obvious that a Monte Carlo scheme based on Eq. (9) will not find a reward at the $x = L$ boundary. The termination at this boundary is based on a finite-difference based representation of the Neumann boundary condition [3] and the random-walker is either absorbed or reflected back into the problem domain. If the random walker is reflected back in the problem domain, once again random walks are generated based on Eq. (9). This partial reflection at the boundary increases the computational time and as a result, Monte Carlo solutions for Neumann and mixed boundary condition problems are considered computationally inefficient. In addition, for the estimation of the derivative, the solution has to be evaluated at multiple points. For this simple one-dimensional problem, one has to obtain the solution at two points, one on each side of the point of interest. These points have to be close enough so that the validity of the first-order approximation for the derivative operator is justified. The actual difference between the solutions at these two points has to be at least an order of magnitude higher than the statistical error in the estimation of the solution. This by itself requires that the number of random walks per solution has to be increased by at least two orders of magnitude as the error is inversely proportional to the square root of the number of random walks [1]. In the newly-developed algorithm, identical amount of computational resources is needed irrespective of whether we are trying to estimate the solution or the derivative. As a result the algorithm is an important first step in the development of computationally efficient GFMC algorithms for Neumann and mixed boundary condition problems.

3. The newly-developed algorithm

As mentioned in the abstract, this algorithm has been inspired by the work of K.K. Sabelfeld [4], where he laid out the spherical mean value relations for the solution and its derivatives in the case of the harmonic and the biharmonic equations. In order to formulate such mean value relations, we proceeded to construct Green's functions whose boundary conditions mimicked the boundary conditions of interest and formulated algorithms for the one-dimensional Laplace equation, the Helmholtz equation and the modified Helmholtz equation [5,6] the details of which are briefly described below. We consider the one-dimensional Helmholtz equation given by

$$\frac{d^2U}{dx^2} + k^2 U = 0, \tag{11}$$

where U is the dependent variable of interest defined in the problem domain $0 \le x \le L$, and k is a complex parameter independent of x. The boundary conditions imposed are $U(0) = \chi$ and $\{dU/dx\}_{x=L} = \delta$. Our approach is motivated by the one-dimensional version of Green's integral representation given by Eq. (4) and is based on a Green's function $G(x|x_0)$ of Eq. (11) given by

$$\frac{d^2G}{dx^2} + k^2 G(x|x_0) = \delta(x - x_0), \tag{12}$$

defined in the problem domain $-h \le x \le h$ with the boundary conditions $G(-h|x_0) = 0$ and $\{dG/dx\}_{x=h} = 0$. This Green's function is explicitly given by

$$\begin{aligned} G(x|x_0) &= -\frac{\cos[k(x_0 - h)]}{k\cos[2kh]} \times \sin\big[k(x + h)\big], \quad x \le x_0, \\ G(x|x_0) &= -\frac{\sin[k(x_0 + h)]}{k\cos[2kh]} \times \cos\big[k(x - h)\big], \quad x \ge x_0. \end{aligned} \tag{13}$$

The boundary conditions that have been imposed on the Green's function given by Eq. (13) and the one-dimensional Green's integral representation given by Eq. (4) have been used to obtain a representation of the solution $U(x_0)$ at a point x_0 within the domain $-h \le x_0 \le h$, and given by

$$U(x_0) = -\left[G(x|x_0)\frac{dU}{dx}\right]_{x=h} - \left[U(x)\frac{dG}{dx}\right]_{x=-h}. \tag{14}$$

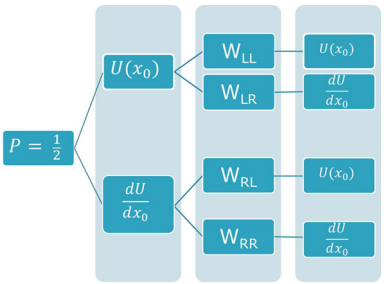

Fig. 1. The schematic for the generation of random-walks.

We now obtain a derivative of Eq. (14) with respect to x_0 and obtain a representation of the derivative of the variable of interest $U(x_0)$ given by

$$\frac{dU}{dx_0} = -\left[\frac{dG}{dx_0}\frac{dU}{dx}\right]_{x=h} - \left[U(x)\frac{d^2G}{dxdx_0}\right]_{x=-h}. \tag{15}$$

Equations (14) and (15) are used to generate a philosophically different Monte Carlo scheme than the one laid out in (2). In order to estimate the solution at a given point, the random walker hops to either the left or the right with probability 1/2 as given by Eq. (14). If the random walker moves to the left, there is a multiplicative weight factor given by $W_{LL} = [-2G_x(x|x_0)]_{x=-h}$ and Eq. (14) is again used to generate the next hop. On the other hand, if the random walker moves to the right, there is a multiplicative weight factor given by $W_{LR} = [-2G(x|x_0)]_{x=h}$ and Eq. (15) is used to generate the next hop. As Eq. (15) is used to generate the random walks, the random walker moves to the left or the right with probability 1/2. If the random walker moves to the left, there is a multiplicative weight factor given by $W_{RL} = [-2G_{xx_0}(x|x_0)]_{x=-h}$ and Eq. (14) is used to generate the next hop. On the other hand, if the random walker moves to the right, there is a multiplicative weight factor given by $W_{RR} = [-2G_{x_0}(x|x_0)]_{x=h}$ and Eq. (15) is used to generate the next hop. A particular random walk terminates either in the left boundary with a reward χ or at the right boundary with a reward δ, and an estimate of the solution is obtained by averaging over a statistically significant number of random walks. Thus, through the use of the Green's function in Eq. (13), the partially reflecting boundary at $x = L$ is converted to an absorbing boundary and there is no reflection. A schematic for the generation of random-walks is given in Fig. 1.

4. Extension of the algorithm to the estimation of derivatives

In this section, we adapt the algorithm to the estimation of the derivative of the solution of the Helmholtz equation. The algorithmic scheme is similar, but the roles of Eqs. (14) and (15) are interchanged. As a result, the random-walk scheme starts with Eq. (15) and not Eq. (14). In order to estimate the solution at a given point, the random walker hops to either the left or the right with probability 1/2 as given by Eq. (15). If the random walker moves to the left, there is a multiplicative weight factor given by $W_{RL} = [-2G_{xx_0}(x|x_0)]_{x=-h}$ and Eq. (14) is used to generate the next hop. On the other hand, if the random walker moves to the right, there is a multiplicative weight factor given by $W_{RR} = [-2G_{x_0}(x|x_0)]_{x=h}$ and Eq. (15) is again used to generate the next hop. If Eq. (14) is used to generate the random walks, the random walker again moves either to the left or to the right with probability 1/2. If the random walker moves to the left, there is a multiplicative weight factor given by $W_{LL} = [-2G_x(x|x_0)]_{x=-h}$ and Eq. (14) is used to generate the next hop. On the other hand, if the random walker moves to the right, there is a multiplicative weight factor given by $W_{LR} = [-2G(x|x_0)]_{x=h}$ and Eq. (15) is used to generate the next hop. As in the case of the estimation of solution, a particular random walk terminates either in the left boundary with a reward χ or at the right boundary with a reward δ, and an estimate of the derivative is obtained by averaging over a statistically significant number of random walks. As a result, there is no reflection and the derivative of the solution can be estimated at any point on the problem domain irrespective of any other point.

In the next section, I will present the results for six representative benchmark problems. However, before that, I would like to take this opportunity to refer to G.A. Mikhailov's very authoritative work [7] on the subject of estimating the derivatives of the solution of boundary value problems through the use of "weighted" Monte Carlo methods. In this approach, relevant Markov chains are formulated and appropriate functionals are estimated from the use of these weights, and subsequent to each transition, the weights show up as multiplicative factors to the ratio of the integral equation kernel and the transition density function. The method allows for the estimation of functionals such as derivatives and G.A. Mikhailov's work sketches out solutions for problems with Dirichlet boundary conditions in great detail. The subject of this work is the estimation of derivatives subject to Neumann and mixed boundary conditions and I believe that it would be an extremely interesting extension of this research to develop weighted Monte Carlo approaches subject to Neumann and mixed boundary conditions.

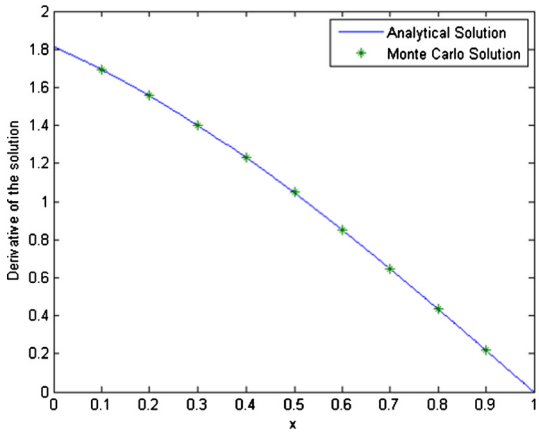

Fig. 2. Derivative of the solution plotted against length for $k = \pi/3$, $L = 1$, $\chi = 1$, $\delta = 0$.

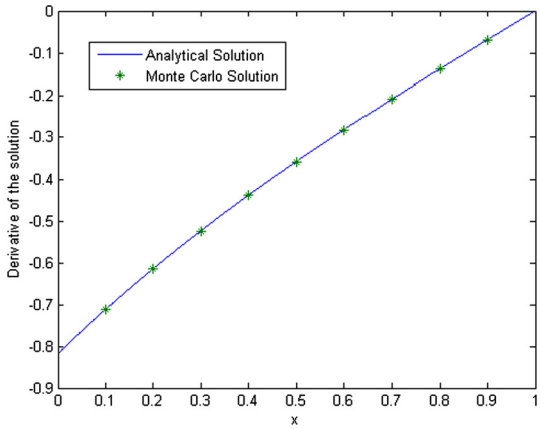

Fig. 3. Derivative of the solution plotted against length for $k = i(\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 0$.

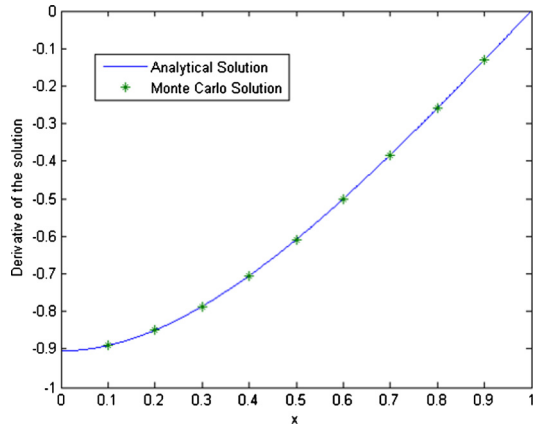

Fig. 4. Real part of the derivative of the solution plotted against length for $k = (1+i)(\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 0$.

5. Results

The benchmark problems are chosen with representative values of L, k, χ and δ and 10^6 random walks were used for the estimation of the derivative at each point. Based on Figs. 2 to 9 and Table 1, it is obvious that the analytical and random walk results are in extremely good agreement, thereby validating the application of our newly developed algorithm. The algorithm is tested in two limiting cases. In one limit, the derivative of the solution on the right boundary is zero and in the other limit, the derivative of the solution on the right boundary is chosen to be 10, a fairly large number. The

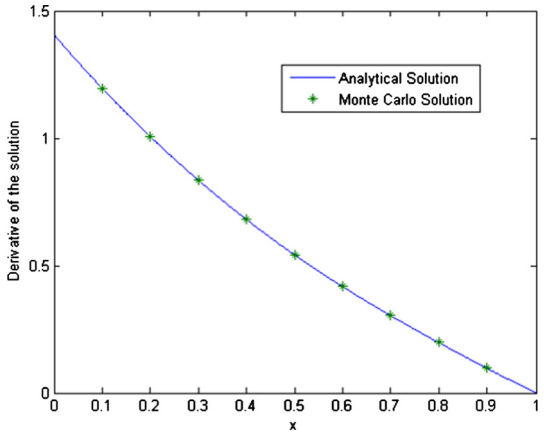

Fig. 5. Imaginary part of the derivative of the solution plotted against length for $k = (1+i)(\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 0$.

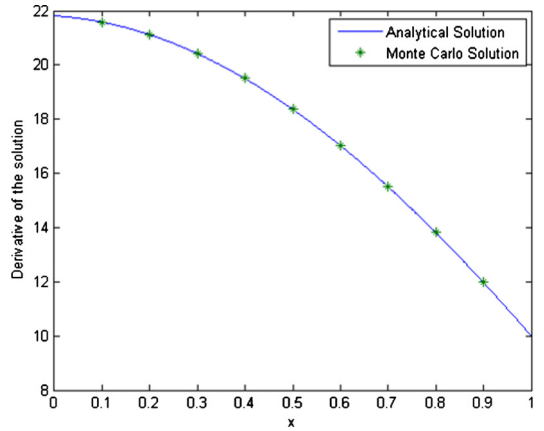

Fig. 6. Derivative of the solution plotted against length for $k = \frac{\pi}{3}$, $L = 1$, $\chi = 1$, $\delta = 10$.

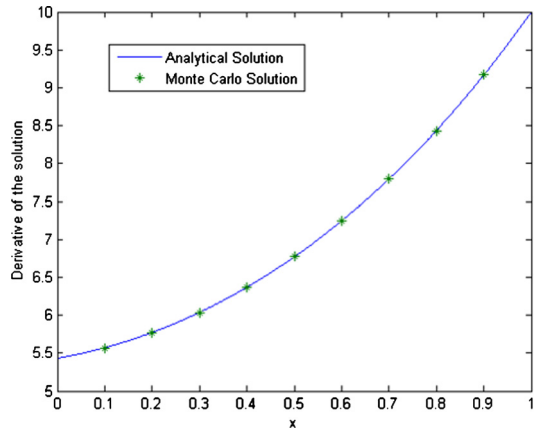

Fig. 7. Derivative of the solution plotted against length for $k = (\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 10$.

algorithm works well in either one of these limits, even though the error in the second limit is higher, which is to be expected. In the second limit, the random-walker receives non-zero contributions when it reaches either of the boundaries and as a result, the statistical error should be higher. Problems (1) to (3) involve three representative problems where the "k-parameter" is real, imaginary and complex and the derivative of the solution at the right boundary is specified to be zero. For these three problems, the exact errors based on deviation from the analytical solution and statistical errors in the solution were both seen to be of the order of 10^{-4}. For problems (4) to (6), the "k-parameters" have the same values as in problems (1) to (3) respectively, but the derivative of the solution was specified to be ten, and for all six problems the

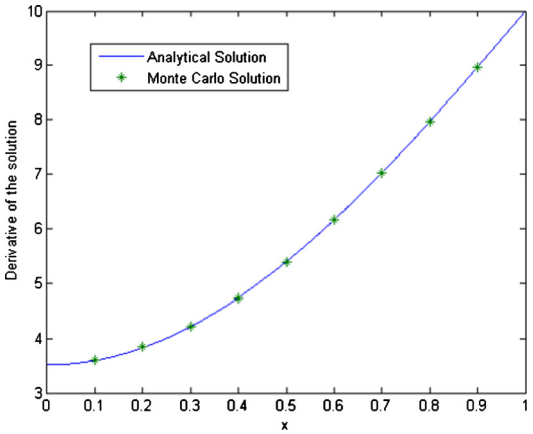

Fig. 8. Real part of the derivative of the solution plotted against length for $k = (1+i)(\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 10$.

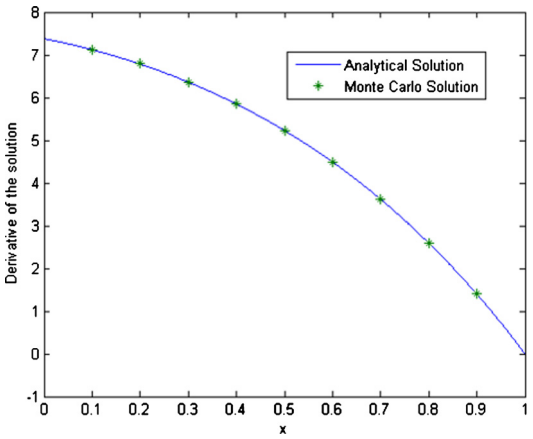

Fig. 9. Imaginary part of the derivative of the solution plotted against length for $k = (1+i)(\pi/3)$, $L = 1$, $\chi = 1$, $\delta = 10$.

Table 1
Comparison of the absolute values of the statistical error and the actual error.

Problem ≠	Parameters	Statistical error	Actual error
1.	$k = \frac{\pi}{3}$, $L = 1$, $\chi = 1$, $\delta = 0$	5.94×10^{-4}	4.85×10^{-4}
2.	$k = \frac{\pi i}{3}$, $L = 1$, $\chi = 1$, $\delta = 0$	1.71×10^{-4}	8.42×10^{-5}
3.	$k = \frac{\pi}{3}(1+i)$, $L = 1$, $\chi = 1$, $\delta = 0$	4.62×10^{-4}	3.80×10^{-4}
4.	$k = \frac{\pi}{3}$, $L = 1$, $\chi = 1$, $\delta = 10$	0.0078	0.0065
5.	$k = \frac{\pi i}{3}$, $L = 1$, $\chi = 1$, $\delta = 10$	0.0038	0.0038
6.	$k = \frac{\pi}{3}(1+i)$, $L = 1$, $\chi = 1$, $\delta = 10$	0.0043	0.0037

solution at the left boundary was assigned the value one. As explained before, the statistical error for problems (4) to (6) were of the order of 10^{-3}, an order of magnitude higher than in problems (1) to (3). However, strong agreement between the exact analytical solutions and Monte Carlo results for all six benchmark problems provides ample validation for this newly-developed methodology.

On another note, the convergence of the algorithm can be guaranteed by ensuring the finiteness of the mean and the variance of the relevant estimator. For the sake of simplicity, we look at the solution of the center of the problem domain for a test problem where $\chi = 1$ and $\delta = 1$. The random-walker in this case either hops to the left or to the right and terminates either on the left boundary where the solution is known or on the right boundary where the derivative of the solution is known. Based on Eq. (15) and using a zero-centered notation in a problem domain extending from $-h \leq x \leq h$, we define a random variable associated with the estimator given by

$$Z = \begin{cases} -2G_{x_0}(h|0) & \text{with probability } 1/2 \\ -2G_{xx_0}(-h|0) & \text{with probability } 1/2 \end{cases} \tag{16}$$

As a result, the mean and variance of the estimator is given by

$$Mean(Z) = \frac{\cos(kh) + \sin(kh)}{\cos(2kh)}, \qquad Variance(Z) = \frac{1 - 2\sin(kh)\cos(kh)}{\cos^2(2kh)}. \tag{17}$$

The finiteness of the mean and the variance is ensured by restricting the size of the problem domain to less than quarter-wavelength length scales, i.e., $Real(2\text{kh} < \pi/2)$. This, in turn, means that the restriction that the real part of kL is less than $\pi/2$ is a sufficient condition for the convergence of the algorithm. This problem with the associated constraint is present not just for Neumann and mixed boundary condition problems, but for Dirichlet problems as well. However within that constraint, excellent agreement has been obtained between the analytical solutions and the numerical results.

The error in the algorithm is statistical in nature and inversely proportional to the square root of the number of random walks [1] which in turn is proportional to the surface area of the problem domain:

$$E \propto \frac{1}{\sqrt{N}} \propto \frac{1}{L^{(n-1)/2}}, \tag{18}$$

where E is the error, N is the number of random walks, L is the size parameter of the problem domain and n is the dimensionality of the problem domain. The number of hops per random walk can also be approximately estimated based on the dimensionality of the problem domain. Assuming the problem domain to be a line, square and a cube in one, two and three dimensions respectively, the probability that the random walker converges to a problem boundary in any given walk is given by

$$p = \frac{1}{2n} \tag{19}$$

where p is the probability of convergence and n is the dimensionality of the problem domain. Thus, the average number of hops per random walk is given by

$$S = \sum_{r=1}^{\infty} r(1-p)^{r-1}p. \tag{20}$$

Substituting $x = 1 - p$, S is given by

$$S = \sum_{r=1}^{\infty}\left(rx^{r-1} - rx^{r}\right) = (1-x)\sum_{r=1}^{\infty} rx^{r-1} = (1-x)\frac{d}{dx}\sum_{r=1}^{\infty} x^{r} = (1-x)\frac{1}{(1-x)^2} = \frac{1}{1-x} = \frac{1}{p}. \tag{21}$$

It can be seen from Eq. (21), the average number of hops per random walk in one, two and three dimensions is two, four and six respectively, and thus Eq. (21) together with Eq. (18) provides an order of magnitude estimate as to how the statistical error would scale if the method is extended to two and three dimensions.

6. Conclusion

Summarizing, a newly-developed GFMC algorithm [5,6] for Neumann and mixed boundary problems has been adapted to the estimation of the derivative of the solution of the 1D Helmholtz equation. In this algorithm, reflecting boundaries are converted into absorbing boundaries through the development of Green's functions that mimic the boundary conditions of the problem of interest. The GFMC results have been benchmarked by an exact analytical solution. The extension of the algorithm to the estimation of the derivative of the solution of the PDE is of immense practical significance, as the derivative of the solution is often needed in physical applications. Examples of such applications include the estimation of electric and magnetic field in electromagnetic problems or the rate of change of temperature in heat conduction problems. My future work in this area will involve the extension of this algorithm to both frequency and time-domain problems in two and three dimensions as well as the development of weighted Monte Carlo approaches for boundary value problems subject to Neumann and mixed boundary conditions. The long-term goal of this research is the application of this methodology to the numerical solution of the F region ionization problem in space plasma modeling [8].

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