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A Green's function Monte Carlo algorithm for the Helmholtz equation subject to Neumann and mixed boundary conditions: Validation with an 1D benchmark problem

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Abstract. In this paper, we present the application of our recently developed Green's function Monte Carlo algorithm to the solution of the one-dimensional Helmholtz equation subject to Neumann and mixed boundary conditions problems. The traditional Green's function Monte Carlo approach for the solution of partial differential equations subjected to Neumann and mixed boundary conditions involves "reflecting boundaries" resulting in relatively large computational times. Our algorithm, motivated 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. In the past, we have applied it to the solution of the one-dimensional Laplace equation and the modified Helmholtz equation. In this work, we apply it to the solution of the Helmholtz equation. In the case of the Helmholtz equation, unlike the Laplace equation and modified Helmholtz equation, the algorithm is constrained to quarter-wavelength length scales, a constraint that is the result of resonance in the Green's function for the Helmholtz equation. This constraint is also present in the case of the Helmholtz equation subjected to Dirichlet conditions and is not specific to Neumann and mixed boundary conditions. However, within this constraint, excellent agreement has been obtained between an analytical solution and numerical results.

Keywords. Green's function Monte Carlo, floating random walk, Helmholtz equation, parallelizable algorithm.

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1 Introduction

We consider a differential equation, with a differential operator L,

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

where the solution $U(x)$ is a function of the one-dimensional position vector x defined in the region $a \leq x \leq b$. The function $f(x)$ is the forcing function. The

Green's functions for (1) are the solutions of the differential equation

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

subject to specified boundary conditions. We assume that the operator L is of the Sturm–Liouville [3] form

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

where $p(x)$ and $q(x)$ are known functions of x. Using Green's integral representation [3], $U(x)$ can be written as

$$U(x_0) = \int_a^b f(x_0)G(x|x_0)dx_0 + \left[u(x)\frac{dG(x|x_0)}{dx}\right]_a^b + \left[G(x|x_0)\frac{dU(x)}{dx}\right]_a^b. \tag{4}$$

The first term on the right-hand side of (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 the 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 of (4) reduces to

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

In problems with inhomogeneous Dirichlet boundary conditions, the random walker finds a reward in each of the 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 traditional Monte Carlo literature [4], these boundary conditions are formulated as partially "reflecting" as the random walker has a chance of either being absorbed in the problem boundary or being thrown back into the problem domain. We will now explain this issue of reflection within the context of 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 $0 \leq x \leq L$. The boundary conditions imposed on this problem are $U(0) = \alpha$ and

$U(L) = \beta$. A traditional Green's function Monte Carlo 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 $-h \leq x \leq h$, with homogeneous Dirichlet boundary conditions $G(-h|x_0) = 0$ and $G(+h|x_0) = 0$. The solution to (7) in a zero-centered notation (i.e., $x_0 = 0$) is given by

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

Based on the 1D version of the Green's integral representation (5) with homogeneous Dirichlet boundary conditions being imposed on the Green's function, the solution to (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 Green's function Monte Carlo algorithm, (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 $0 \leq x \leq L$ 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 is N_α and N_β, respectively. Now let us consider the solution of (6) defined on the problem domain $0 \leq x \leq L$, but with the boundary conditions $U(0) = \alpha$ and $\{dU/dx\}_{x=L} = \beta$. It is obvious that a Monte Carlo scheme based on (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 [4] 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 (9). This partial reflection at the boundary increases the computational time and, as a result, Neumann and mixed boundary condition problems are considered difficult to be handled with the Monte Carlo method, particularly for problem domains in 2D and 3D with complicated geometries. We will now discuss our recently developed algorithm, where this requirement for reflection is eliminated.

3 The newly developed algorithm

As mentioned in the abstract, this algorithm has been motivated by the work of K. K. Sabelfeld [5], 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 and the modified Helmholtz equation [1, 2]. In this paper, we use this approach to develop a Monte Carlo algorithm for the one-dimensional Helmholtz equation given by

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

where U is the dependent variable of interest defined in the problem domain $0 \leq x \leq L$, and k is a real number 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 (4) and is based on a Green's function $G(x|x_0)$ of (11) given by

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

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

$$G(x|x_0) = \begin{cases} -\frac{\cos[k(x_0-h)]}{k\cos[2kh]}\sin[k(x+h)], & x \leq x_0, \\ -\frac{\sin[k(x_0+h)]}{k\cos[2kh]}\cos[k(x-h)], & x \geq x_0. \end{cases} \tag{13}$$

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

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

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

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

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 (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 (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 (15) is used to generate the next hop. As (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 (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 (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 (13), the partially reflecting boundary at $x = L$ is converted to an absorbing boundary and there is no reflection. The schematic for the generation of the random walks is shown in Figure 1.

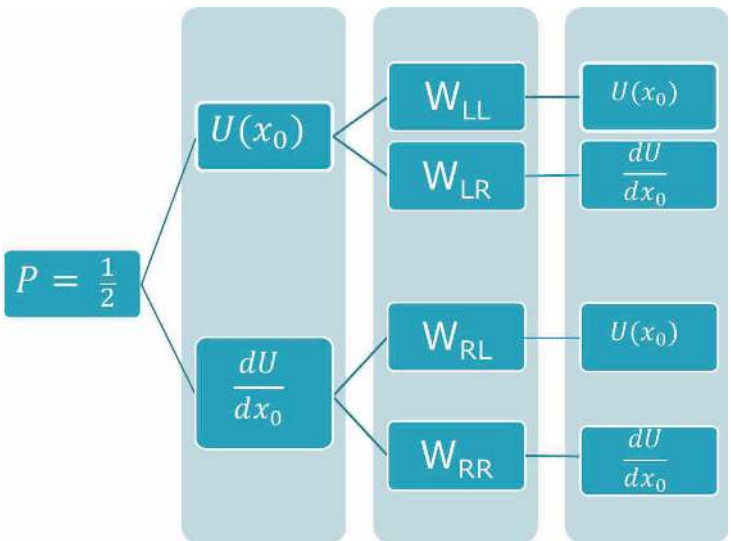

Figure 1. The schematic for the generation of random walks.

4 Results

A mixed boundary condition problem for the Helmholtz equation given by (11) is chosen with representative values of L, k, χ and δ. In the Monte Carlo simulations, 2×10^6 random walks have been carried out for each solution point and the average error between the analytical results and the Monte Carlo solutions was seen to be around 0.1 percent.

We finish our discussion on the formulation of the algorithm with a note on its convergence, which is 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 $k = 1$, $\chi = 1$ 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 (14) and using a zero-centered notation in a problem domain extending from $-h \le x \le h$, we define a random variable associated with the estimator given by

$$Z = \begin{cases} -2G(h|0) & \text{with probability } 1/2, \\ -2\frac{dG(-h|0)}{dx} & \text{with probability } 1/2. \end{cases} \tag{16}$$

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

$$\text{Mean}(Z) = E(Z) = \frac{1}{2}\frac{2\sin(h)}{\cos(2h)} + \frac{1}{2}\frac{2\cos(h)}{\cos(2h)} = \frac{\sin(h)+\cos(h)}{\cos(2h)}, \tag{17}$$

$$\begin{aligned} \text{Variance}(Z) &= E(Z^2) - \{E(Z)\}^2 \\ &= \frac{1}{2}\frac{4\cos^2(h)}{\cos^2(2h)} + \frac{1}{2}\frac{4\sin^2(h)}{\cos^2(2h)} - \left\{\frac{1}{2}\frac{2\sin(h)}{\cos(2h)} + \frac{1}{2}\frac{2\cos(h)}{\cos(2h)}\right\}^2 \\ &= \frac{1-2\sin(h)\cos(h)}{\cos^2(2h)}, \end{aligned} \tag{18}$$

where $E(\cdot)$ represents the expectation of a random variable. 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., $2h < \pi/2$. This problem of "quarter-wavelength resonance" for the Monte Carlo solution of the Helmholtz equation is present for the Dirichlet problem as well. But within that constraint, excellent agreement has been obtained between the exact analytical solutions and numerical results, as evidenced by the obtained results.

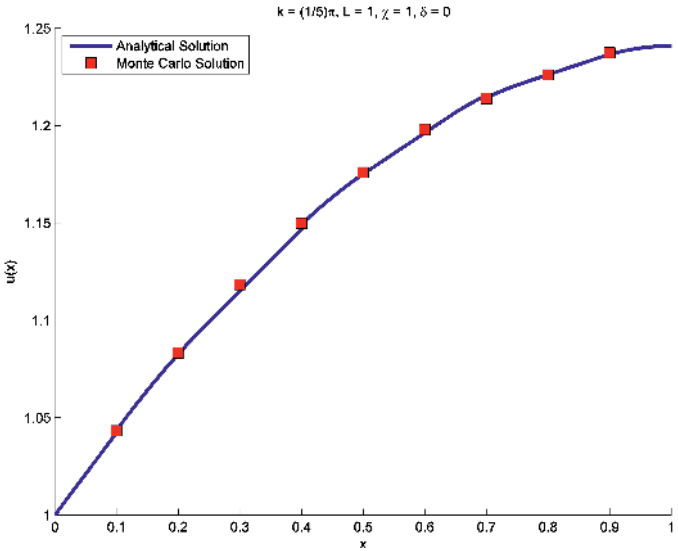

Figure 2. Analytical and Monte Carlo results for the solution of the Helmholtz equation plotted against length for $k = \frac{\pi}{5}$, $L = 1$, $\chi = 1$, $\delta = 0$.

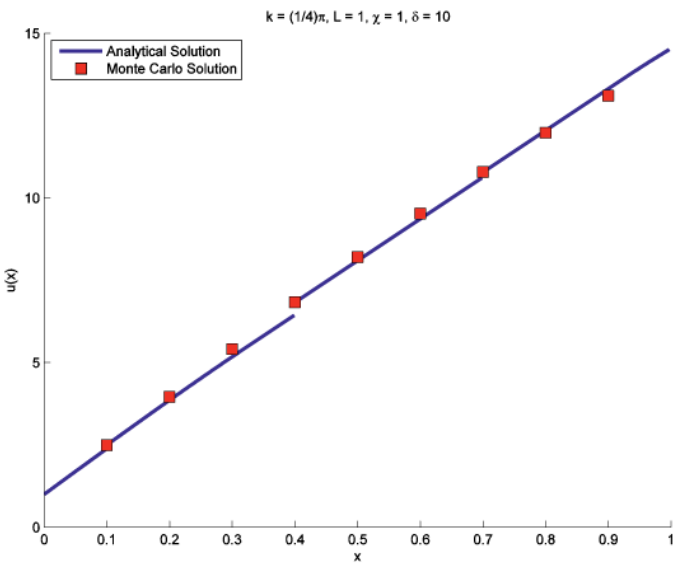

Figure 3. Analytical and Monte Carlo results for the solution of the Helmholtz equation plotted against length for $k = \frac{\pi}{4}$, $L = 1$, $\chi = 1$, $\delta = 10$.

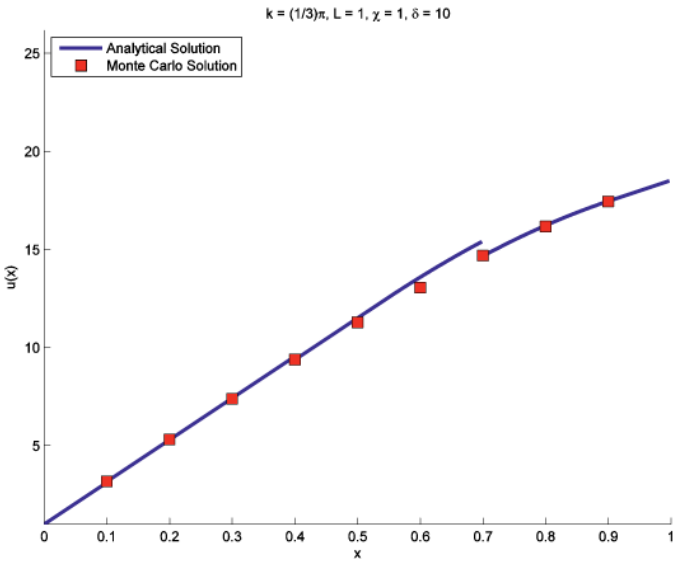

Figure 4. Analytical and Monte Carlo results for the solution of the Helmholtz equation plotted against length for $k = \frac{\pi}{3}$, $L = 1$, $\chi = 1$, $\delta = 10$.

5 Conclusion

Summarizing, a newly developed Monte Carlo algorithm [1, 2] for Neumann and mixed boundary problems has been extended to 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 algorithm has been validated by an analytical solution and excellent agreement has been obtained between analytical and numerical results. Due to the problem of resonance in the Green's function, the algorithm is restricted to quarter-wavelength length scales. Our future work in this area will involve the extension of this algorithm to important equations in time-domain such as the heat equation and to problems in two and three dimensions.

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