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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

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