

Walk-on-spheres algorithm for solving Poisson equation with abrupt material change

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Conventional numerical simulation methods may become challenging when handling complex geometries due to ineffective discretization and large number of degrees of freedom. Based on the integral representation of electric potential derived from Green's theorem, a recursive estimate of the potential can be obtained. The walk-on-spheres algorithm is introduced to solve the Poisson equation when abrupt change of material exists. The proposed method is mesh-free and progressive, which has been validated by comparing the results with conventional methods, showing great potential in handling problems with complex geometries.

Index Terms—Numerical analysis, Monte Carlo methods, Green function, Poisson equations

I. INTRODUCTION

WITHIN the conventional numerical methods, such as the finite element method, the boundary element method, and the finite difference time domain method, the discretization of geometry is often required to solve partial differential equations (PDEs), which would result in inaccurate results and increased computational time when handling complex geometries. Recent developments in computer graphics have introduced the so-called mesh-free Monte Carlo methods for solving PDEs without the need for discretization [1], [2]. In particular, the development of the walk-on-spheres (WoS) algorithm has facilitated its application to the Poisson equation with various boundary condition scenarios, such as Dirichlet [1], Neumann [3], Robin boundary conditions [4], as well as floating potential boundaries [5]. Moreover, the Monte Carlo method is also applicable when handling inhomogeneous material when the gradient of the material change is not too great [2]. Nonetheless, previous WoS algorithms fail when the material properties change abruptly, which is of substantial importance in the fields of electrical engineering and computational electromagnetics. Towards this end, we propose a WoS algorithm for solving Poisson equations with material interfaces, providing a grid-free Monte Carlo solver for multi-medium regions.

II. THEORY AND METHODS

Fig. 1 illustrates a multi-dielectric region of interest, where two regions Ω_1 and Ω_2 are separated by an interface Γ_{12} , with homogeneous dielectric constants being ϵ_1 and ϵ_2 , respectively. The boundary value problem (BVP) with Dirichlet boundary conditions can be expressed as

$$\nabla^2 \varphi_i(\mathbf{x}) = -f_i(\mathbf{x})/\epsilon_i, \quad \mathbf{x} \in \Omega_i (i = 1, 2), \quad (1a)$$

$$\varphi(\mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega_D, \quad (1b)$$

$$\varphi_1(\mathbf{x}) = \varphi_2(\mathbf{x}), \quad \mathbf{x} \in \Gamma_{12}, \quad (1c)$$

$$\mathbf{n}_{12} \cdot \epsilon_2 \nabla \varphi_2(\mathbf{x}) = \mathbf{n}_{12} \cdot \epsilon_1 \nabla \varphi_1(\mathbf{x}), \quad \mathbf{x} \in \Gamma_{12}, \quad (1d)$$

where ∇^2 denotes the Laplacian operator; f_i denotes the charge densities in region Ω_i ; $g(\mathbf{x})$ denotes the known boundary value

on the Dirichlet boundary $\partial\Omega_D = (\partial\Omega_1 \cup \partial\Omega_2) \setminus \Gamma_{12}$; $\Gamma_{12} = \partial\Omega_1 \cap \partial\Omega_2$ denotes the interface between Ω_1 and Ω_2 ; $\mathbf{n}_{12}$ is the unit normal vector pointing from Ω_1 to Ω_2 at Γ_{12} .

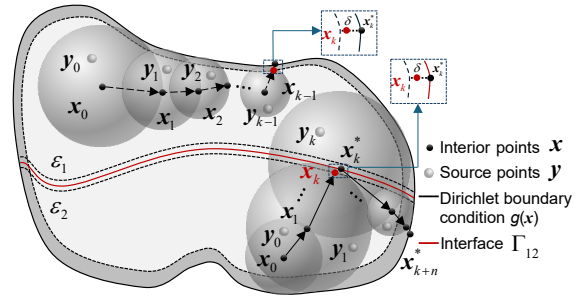


Fig. 1. **Illustration of the walk-on-spheres algorithm for potential.** The line with arrow in Ω_2 represents the random walks that intersect the interfaces, and the Long-dashed line with arrow in Ω_1 denotes the random walks that never intersect the interface and end at the Dirichlet boundaries. Note that the two types of random walk paths would eventually be absorbed by the Dirichlet boundaries in a δ -layer illustrated in the shaded region.

By using Green's theorem, we can derive the integral equations for $\varphi(\mathbf{x})$ in the homogeneous domain and on the interface. Inside the homogeneous domain Ω_i , we have

$$\varphi_i(\mathbf{x}) = \frac{\int_{\partial B_i(\mathbf{x}, R)} \varphi_i(\mathbf{y}) d\mathbf{y}}{|\partial B_i(\mathbf{x}, R)|} + \int_{B_i(\mathbf{x}, R)} G^{B_i(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) \frac{f_i(\mathbf{y})}{\epsilon_i} d\mathbf{y}, \quad (2)$$

where $\varphi_i(\mathbf{x})$ denotes electric potential at $\mathbf{x} \in \Omega_i \setminus \Gamma_{12}$; $G^{B_i(\mathbf{x}, R)}$ represents the Green's function within a ball $B_i(\mathbf{x}, R) \subset \Omega_i$ centered at $\mathbf{x}$ with radius R .

When $\mathbf{x} \in \Gamma_{12}$, the potential $\varphi_i(\mathbf{x})$ can be expressed as

$$\begin{aligned} c_i \varphi_i(\mathbf{x}) &= \int_{\Gamma_{12} \cap [B(\mathbf{x}, R) \setminus B(\mathbf{x}, \gamma)]} g_i [G^{B(\mathbf{x}, R)}, \varphi_i(\mathbf{y})] d\mathbf{y} \\ &+ \frac{1}{|\partial B(\mathbf{x}, R)|} \int_{S^i(\mathbf{x}, R)} \varphi_1(\mathbf{y}) d\mathbf{y} \\ &+ \int_{B^i(\mathbf{x}, R)} G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) \frac{f_i(\mathbf{y})}{\epsilon_i} d\mathbf{y}, \end{aligned} \quad (3)$$

where $c_i = |\partial B(\mathbf{x}, \gamma)|^{-1} \int_{S^i(\mathbf{x}, \gamma)} d\mathbf{y}$ ($c = \theta_i/2\pi$ and $c_i = \theta_i/4\pi$ for 2D and 3D, respectively, with θ_i being the

planar/solid angle (2D/3D) of $S^i(\mathbf{x}, \gamma)$ with respect to Γ_{12} ; $S^i(\mathbf{x}, R|\gamma) = \partial B(\mathbf{x}, R|\gamma) \cap \Omega_i$ and $B(\mathbf{x}, R|\gamma)$ is the ball centered at $\mathbf{x}$ on the interface with radius $R|\gamma$ ($\gamma \ll R$); $g_i \left[G^{B(\mathbf{x}, R)}, \varphi_i(\mathbf{y}) \right] = G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) (-1)^i \mathbf{n}_{21} \cdot \nabla_{\mathbf{y}} \varphi_i(\mathbf{y}) - \varphi_i(\mathbf{y}) (-1)^i \mathbf{n}_{21} \cdot \nabla_{\mathbf{y}} G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y})$ and the partial ball $B^i(\mathbf{x}, R) = B(\mathbf{x}, R) \cap \Omega_i$. By inserting (3) into the boundary conditions (1d), one can obtain the solution of $\varphi(\mathbf{x})$ on the interface as

$$\begin{aligned} c\varphi(\mathbf{x}) = & \xi_1 \int_{S^1(\mathbf{x}, R)} \frac{\varphi(\mathbf{y})}{|\partial B(\mathbf{x}, R)|} d\mathbf{y} + \xi_2 \int_{S^2(\mathbf{x}, R)} \frac{\varphi(\mathbf{y})}{|\partial B(\mathbf{x}, R)|} d\mathbf{y} \\ & + (\xi_2 - \xi_1) \oint_{\Gamma_{12} \cap B(\mathbf{x}, R)} \varphi(\mathbf{y}) \mathbf{n}_{12} \cdot \nabla_{\mathbf{y}} G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) d\mathbf{y}, \\ & + \xi_1 \int_{B^1(\mathbf{x}, R)} G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) f_1(\mathbf{y}) d\mathbf{y} \\ & + \xi_2 \int_{B^2(\mathbf{x}, R)} G^{B(\mathbf{x}, R)}(\mathbf{x}, \mathbf{y}) f_2(\mathbf{y}) d\mathbf{y} \end{aligned} \quad (4)$$

where $\oint \bullet d\mathbf{y}$ denotes the principal value integral since ∇G^B would become singular when $\mathbf{y}$ approaches $\mathbf{x}$; $\xi_i = \varepsilon_i / (\varepsilon_1 + \varepsilon_2)$ for $i = 1, 2$.

Having derived the integral equations of the potential, we move on to the implementation of Monte Carlo estimation of (4) within the WoS algorithm. Since an integral can be estimated by using the Monte Carlo method, the randomization of (2) and (4) leads to the estimate based on the simulation of the walk-on-spheres Markov chain. Therefore, the recursive estimate of $\varphi(\mathbf{x})$ can be expressed as

$$\hat{\varphi}(\mathbf{x}_k) = \begin{cases} \hat{\varphi}(\mathbf{x}_{k+1}), & d_k > \delta, \\ g(\mathbf{x}_k^*), & d_k < \delta, \quad \mathbf{x}_k^* \in \partial\Omega_D, \\ \hat{\varphi}_{12}(\mathbf{x}_k^*), & d_k < \delta, \quad \mathbf{x}_k^* \in \Gamma_{12}, \end{cases} \quad (5)$$

where $\hat{\varphi}$ and $\hat{\varphi}_{12}$ are the sampled estimators of the potential in the homogeneous domain (Ω_1 or Ω_2) and on the interface Γ_{12} , respectively; $\mathbf{x}_{k+1} \in \partial B(\mathbf{x}_k, R)$ denotes a uniform random point on the boundary of $B(\mathbf{x}_k, R)$; $d_k = |\mathbf{x}_k - \mathbf{x}_k^*|$ is the shortest distance to the domain boundaries and $\mathbf{x}_k^*$ is the corresponding closest point on the boundaries. As illustrated in Fig. 1, the random walk starts from an arbitrary point $\mathbf{x}_0$ and terminates at $\mathbf{x}_k$ when $\mathbf{x}_k$ is located within a small distance $\delta > 0$ from the domain boundary (i.e., $d_k < \delta$). When the point $\mathbf{x}_k$ is located within a small distance $\delta > 0$ from the interface Γ_{12} , the random walk will continue and $\hat{\varphi}_{12}(\mathbf{x}_k^*)$ can be determined by the subsequent walk's location according to (4). The pseudocode of WoS algorithms is summarized in Algorithm 1.

III. RESULTS AND DISCUSSIONS

Fig. 2 depicts the relative error between the Monte Carlo method and the analytical solution for a two-layer-insulated coaxial cable. As the number of random walks N is increased, the results converge, indicating that the proposed mesh-free WoS algorithm is a progressive approach akin to rendering in computer graphics. However, the random walks may adhere to the interface, resulting in extended walk durations. A possible solution to address this issue may be deliberately sampling the next points on spheres with a radius as large as possible when the points of interest or the random walks arrive at or near

Algorithm 1 Walk-on-sphere (WoS) algorithm for Laplace equation with abrupt material change and flat interfaces.

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1:  $\varphi = 0$  ▷ solution estimate
2: for  $i \leftarrow 1$  to  $N$  do ▷  $N$  is the number of random walks
3:    $\mathbf{x} = \mathbf{x}_0$  ▷ point of interest
4:    $N_1 = N_2 = 0$  ▷ # of walks in  $\Omega_i$  originated from interface
5:   while  $l_D > \delta$  do ▷ start a new walk
6:      $l_D = \text{distanceToDirichlet}(\mathbf{x}, \partial\Omega_D)$ 
7:      $l_{12} = \text{distanceToInterface}(\mathbf{x}, \Gamma_{12})$ 
8:      $d = \min(l_{12}, l_D)$  ▷ distance to all boundaries
9:      $\mathbf{x} = \text{randomSphere}(\mathbf{x}, d)$  ▷ random point on sphere
10:    if  $l_{12} < \delta$  and  $\mathbf{x} \in \Omega_i$  then ▷ points near interface
11:       $N_i++$  ▷  $i = 1, 2$ 
12:    end if
13:  end while
14:   $\varphi += g(\mathbf{x}) \cdot \xi_1^{N_1} \xi_2^{N_2}$ 
15: end for
16: return  $\varphi/N$  ▷ return average boundary value

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the interface. Moreover, future works may focus on the more efficient implementation of the algorithm when the interface is not flat or multiple interfaces intersect.

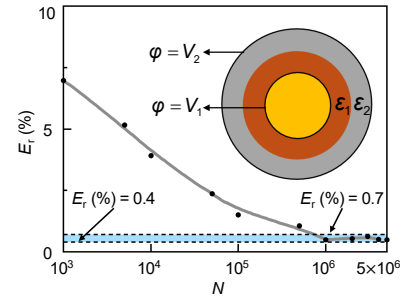


Fig. 2. **Relative error as a function of the number of random walks.** The inset shows the structure of the partially simplified model of a coaxial cable. Here, $E_r = \|\varphi_{\text{WoS}} - \varphi_{\text{exact}}\|_2 / \|\varphi_{\text{exact}}\|_2$, where φ_{WoS} and φ_{exact} are the potential calculated within WoS and analytical solution, respectively.

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