A Novel Dirichlet-Neumann Random-Walk Algorithm for the Solution of Time-Harmonic Helmholtz Equation at Multiple Wavelength Length Scales: 1D and 2D Verification

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Abstract: The electrical properties of IC interconnects at multi-GHz frequencies must be described with Maxwell's equations. We have created an entirely new floating random-walk (RW) algorithm to solve the time-harmonic Maxwell-Helmholtz equations. Traditional RW algorithms for Maxwell-Helmholtz equations are constrained to length scales that are less than a quarter-wavelength. This is because of the problem of resonance in finite-domain Green's function for Helmholtz equation at multiple quarter-wavelength length scales. In this paper, we report the major discovery of extending our floating RW algorithm beyond a quarter-wavelength. The problem of Green's function resonance has been eliminated by the use of an infinite-domain Green's function. In this work, we formulate this algorithm and describe its successful application to homogeneous and heterogeneous 1D problems and homogeneous 2D problems. We believe, that with additional work, this RW algorithm will prove useful in the development of CAD tools for electromagnetic analysis of IC interconnect systems. It can be noted that the algorithm exhibits full parallelism, requiring minimal interprocessor communication. Thus, significant performance enhancement can be expected in any future parallel software or hardware implementation.

Keywords: Floating random-walk method/algorithm, Dirichlet-Neumann algorithm, Maxwell-Helmholtz equation.

1. Introduction

Fundamentally, the electrical properties of advanced multilevel IC interconnects at present multi-GHz frequencies must be described with Maxwell's equations. Traditional numerical methods[1-3] require, usually, a discretization mesh. Mesh size and resultant difficulty of solution become somewhat unmanageable in complicated 3D problem domains. The RW algorithm that we present here does not involve the use of a mesh. In essence, the algorithm executes a Monte Carlo integration [4] of an infinite series of multi-dimensional integrals [5] by means of random walks (RWs) through the problem domain. These integrals contain both "surface" and "volume" Green's function kernels. Conventional RW algorithms for Maxwell-Helmholtz equation are constrained to sub-quarter-wavelength length scales. This is due to the mathematical difficulties associated with unwanted multiple quarter-wavelength resonances [6] in finite-domain Green's functions. In this work, the problem of finite-domain Green's function resonance has been eliminated by the use of an infinite-domain Green's function. The additional complexity of having now to propagate RWs for both the field and its derivative presents little practical difficulty. In the next section, we present the RW equations for the time-harmonic Maxwell-Helmholtz equations in 1D and 2D.

2. Random-Walk Equations

Consider the 1D time-harmonic Maxwell-Helmholtz equation with a source term on the right-hand side

$$\frac{d^2 A(x)}{dx^2} + k^2 A(x) = f(x). \tag{1}$$

The quantity A is the field variable of interest and k is a constant wave vector whose magnitude is determined by the frequency and material properties of the problem domain. Both the boundary value and derivative are assumed to be known at the two endpoints of the 1D problem domain. Now, one may wonder why we want to solve an "over-specified" problem. This criticism can be countered by observing that in IC-interconnect structures, the current is specified at certain conducting regions. These currents appear as source terms in the right hand side of the Helmholtz equation given in (1). Integrals involving these source terms will appear in our RW formulation and the RWs will terminate at infinity, that is, at large distances from the interconnect structure, where the field vector of interest and its spatial derivatives are known to be zero from physical considerations. The non-zero contributions to the RW solution will come from integrals involving source terms. So, having established the motivation for solving the 1D problem of interest, we can write the Green's function differential equation associated with (1)

$$\frac{\partial^2 G(x \mid x_o)}{\partial x^2} + k^2 G(x \mid x_o) = \delta(x - x_o), \tag{2}$$

where $\delta(x-x_0)$ is the Dirac delta function centered at $x = x_o$. There can be any number of Green's functions satisfying equation (2), depending on the arbitrary nature of boundary conditions applied to (2). In a previous work[6], we have employed one such finite-domain Green's function that vanishes at problem-domain boundaries For instance, over $-L \le x \le L$, such a Green's function has the form

$$G(x \mid x_{\mathbf{o}}) = \frac{1}{2k\cos kL}\sin\left[k\left(\mid x - x_o \mid - L\right)\right]. \tag{3}$$

The use of a finite-domain Green's function like the one in (3) produces the most economical set of RW equations, and is traditional in RW literature. On the other hand, it is precisely this form of the finite-domain Green's function that generates unwanted multiple quarter-wavelength resonance, produced by the zeros in the denominator of (3).

In this work, we suggest the use of an infinite-domain Green's function, where both the boundary value and the boundary derivative never simultaneously vanish at domain boundaries. One such Green's function satisfying (2) is, for example,

$$G(x \mid x_{\mathbf{o}}) = \frac{1}{2k}\sin\left(k \mid x - x_o \mid\right). \tag{4}$$

Using (4), the problem of quarter-wavelength resonance can be avoided, at the minimal expense of now propagating, by RWs, both field values and derivatives through the problem domain. We therefore call this new modification a D-N floating RW algorithm, where "D-N" signifies "Dirichlet-Neumann". To obtain the RW equations, we multiply (1) by $G(x \mid x_o)$ and (2) by $A(x)$ and subtract one from the other, which yields

$$A\frac{d^2G}{dx^2} - G\frac{d^2A}{dx^2} = A\delta(x - x_o) - f(x)G(x \mid x_o). \tag{5}$$

Integrating (5) from $-L$ to $+L$, yields

$$\begin{aligned} A(x_o) = &\int_{-L}^{+L} G(x \mid x_o) f(x) dx + \\ &G_x(L \mid x_o)A(L) - G_x(-L \mid x_o)A(-L) - \\ &G(L \mid x_o)A_x(L) + G(L \mid x_o)A_x(-L). \end{aligned} \tag{6}$$

In the zero-centered notation, meaning $x_o = 0$, (6) can be written as

$$\begin{aligned} \overline{A} = &\int_{-L}^{+L} G(x) f(x) dx + \overline{G}_x(L)A(L) - \\ &\overline{G}_x(-L)A(-L) - \overline{G}(L)A_x(L) + \overline{G}(L)A_x(-L), \end{aligned} \tag{7}$$

where $\overline{G}_x(L) = G_x(L \mid 0), \overline{G}(L) = G(L \mid 0),$ and so forth. Taking a derivative of (6) with respect to x_o , and writing in zero-centered notation, gives

$$\begin{aligned} \overline{A}_{x_o} = &\int_{-L}^{+L} G_{x_o}(x) f(x) dx + \overline{G}_{xx_o}(L)A(L) - \\ &\overline{G}_{xx_o}(-L)A(-L) - \overline{G}_{x_o}(L)A_x(L) + \overline{G}_{x_o}(L)A_x(-L). \end{aligned} \tag{8}$$

Equations (7) and (8) can be written in the vector-matrix form

$$\begin{aligned} \begin{bmatrix} \overline{A} \\ A_{x_o} \end{bmatrix} = &\begin{bmatrix} \int_{-L}^{+L} G(x) f(x) dx \\ \int_{-L}^{+L} G_{x_o}(x) f(x) dx \end{bmatrix} \\ &+ \begin{bmatrix} \overline{G}_x(L) & -\overline{G}(L) \\ \overline{G}_{xx_o}(L) & -\overline{G}_{x_o}(L) \end{bmatrix} \begin{bmatrix} A(L) \\ A_x(L) \end{bmatrix} + \\ &\begin{bmatrix} -\overline{G}_x(-L) & \overline{G}(-L) \\ -\overline{G}_{xx_o}(-L) & \overline{G}_{x_o}(-L) \end{bmatrix} \begin{bmatrix} A(-L) \\ A_x(-L) \end{bmatrix}, \end{aligned} \tag{9}$$

where A and A_x at the center of the domain $x = x_o$, relates to the hop-interval endpoint values at $x = \pm L$. The different derivatives of the infinite-domain Green's function in (4), which shows up in the matrix-equation (9) are given by

$$\overline{G}_x(x) = \frac{1}{2}\cos(k|x|)\mathrm{sgn}(x),$$
$$x \neq 0, \mathrm{sgn}(x) = \begin{cases} -1, x < 0, \\ 1, x > 0, \end{cases} \tag{10a}$$

$$\overline{G}_{x_o}(x) = -\frac{1}{2}\cos(k|x|)\mathrm{sgn}(x),\ x \neq 0, \tag{10b}$$

$$\overline{G}_{xx_o}(x) = \frac{k}{2}\sin(k|x|),\ x \neq 0. \tag{10c}$$

In the 2D case, the infinite-domain Green's function chosen is

$$G(\mathbf{r} \mid \mathbf{r}_0) = \frac{1}{4}Y_o(k|\mathbf{r} - \mathbf{r}_0|). \tag{11}$$

Above, Y_o represents Neumann function of zeroth order. Using the Green's function in (11), we can solve for the 2D Helmholtz equation with an arbitrary forcing function $f(r,\phi)$. Following a procedure identical to the one that led to the derivation of (7) and (8), the field variable A of interest, and its derivative at the center ($r_o = 0$) of a circular domain of radius R are given by

$$\begin{aligned} \overline{A} = & \int_0^R\int_0^{2\pi} f(r,\phi)G(r,\phi \mid r_o,\phi_o)rdrd\phi + \\ & \int_0^{2\pi} RG_r(R,\phi \mid \phi_o)A(\mathbf{r})_{r=R}d\phi - \\ & \int_0^{2\pi} RA_r(R,\phi \mid \phi_o)G(\mathbf{r} \mid \mathbf{r}_0)_{r=R}d\phi. \end{aligned} \tag{12.1}$$

$$\begin{aligned} \overline{A}_{r_o} = & \int_0^R\int_0^{2\pi} f(r,\phi)G_{r_o}(r,\phi \mid r_o,\phi_o)rdrd\phi + \\ & \int_0^{2\pi} RG_{rr_o}(R,\phi \mid \phi_o)A(\mathbf{r})_{r=R}d\phi - \\ & \int_0^{2\pi} RA_r(R,\phi \mid \phi_o)G_{r_o}(\mathbf{r} \mid \mathbf{r}_0)_{r=R}d\phi. \end{aligned} \tag{12.2}$$

Here, subscripts denote differentiation. The different derivatives of the infinite-domain Green's function given in (11) with respect to r and r_o are given by

$$G_r(R,\phi \mid \phi_o) = \frac{k}{4}Y_o'(kR), \tag{13.1}$$

$$G_{r_o}(R,\phi \mid \phi_o) = -\frac{k}{4}Y_o'(kR)\cos(\phi - \phi_o), \tag{13.2}$$

$$G_{rr_o}(R,\phi \mid \phi_o) = -\frac{k^2}{4}Y_o''(kR)\cos(\phi - \phi_o). \tag{13.3}$$

Thus, we have formulated the RW propagation equations for solving the Helmholtz equation in 1D and 2D. In the following section, we will present the results for test problems in 1D and 2D.

3. Benchmark Problems

We have chosen four benchmark problems. The first two problems involve the solution of Helmholtz equation in 1D. The first problem involves the solution of Helmholtz equation in a medium with real propagation constant (k = 1.0) with a sinusoidal (k_f = 1.5) forcing term. A real propagation constant corresponds to insulating medium, while a complex propagation constant corresponds to conducting medium. The analytical solution chosen is proportional to the forcing term. The rationale behind the choice of a sinusoidal forcing term is that any forcing function, piecewise continuous in the problem domain of interest can be decomposed into an infinite sum of sinusoids. The second problem involves a heterogeneous problem domain with a real propagation constant (k = 3.0) on the left and a complex propagation constant (k = 3.0 + 0.4i). An analytical solution of the form $A\sin(kx) + B\cos(kx)$ is imposed on either side of the interface, while maintaining the continuity of the solution and its derivative at the interface. The third and the fourth problem involve the solution of 2D Helmholtz equation in insulating medium. For the third problem, we have chosen a circular cross section whose radius is equal to twice the wavelength in normalized length scales with k = 1. The solution imposed on the problem domain is the Bessel function of zeroth order. For the fourth problem, we have chosen a Fourier mode solution in a square problem domain whose side is equal to four times the wavelength in normalized length scales with k = 1. The field variable of interest A is zero in the top bottom and right boundary line; along the left boundary line A is equal to $\cos(\pi y / L)$, where L represents the length of the side of the square domain with $y = 0$ coinciding with the bottom boundary line. The reason behind choosing such a solution is again that any piecewise continuous boundary condition can be decomposed into infinite number of such Fourier modes.

In order to estimate our field variable, A, of interest, we define RWs to start at the point, where we need to estimate A. The RWs propagate as "hops" of different sizes from the point of interest to the problem boundary, consistent with a stochastic interpretation of (9) and (12). An accurate statistical estimate for A can be obtained by averaging over large number of such RWs.

The results for these problems are shown in Figures (1) to (5). As seen from the figures, there is very good agreement between the analytical and RW results. We also observe that our algorithm has been able to capture multiple wavelengths. In addition, it can be noted that for the heterogeneous 1D problem, the solution is purely oscillatory in dielectric, while the solution is damped in the conductor. This is consistent with the usual skin-effect type behavior expected in conducting medium. We coded the algorithm in MATLAB 5.0™, using a 400-MHz Apple PowerBook G3™ development platform. The computational details are presented in Table (1).

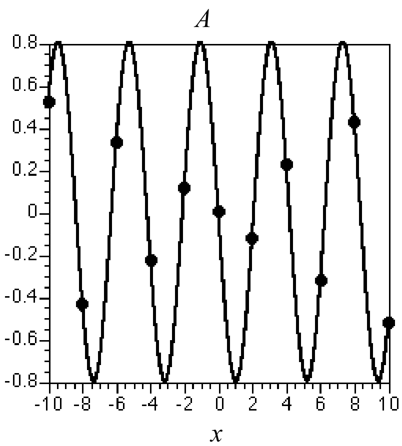

Figure 1: 1D homogeneous problem with real forcing term in insulating medium. -10 ≤ x ≤ 10 in normalized length scales and k = 1. A real, forcing term equal to $\sin(k_f x)$ is applied with $k_f = 1.5$. The solid line represents the exact analytical solution. The dots represent the random-walk solution points.

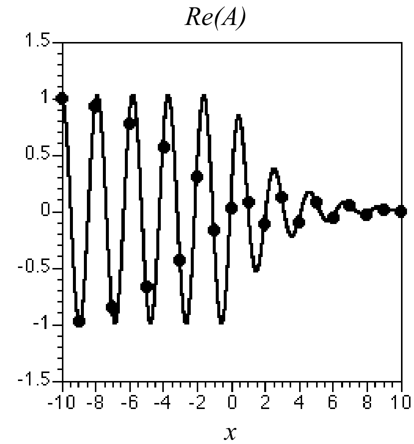

Figure 2: 1D heterogeneous problem, the real part of the solution. Heterogeneous domain with -10 ≤ x ≤ 10 in normalized length scales. For x ≤ 0, k = 3, while for x ≥ 0, k = 3 + 0.4i. The solid line represents the exact analytical solution. The dots represent the random-walk solution points.

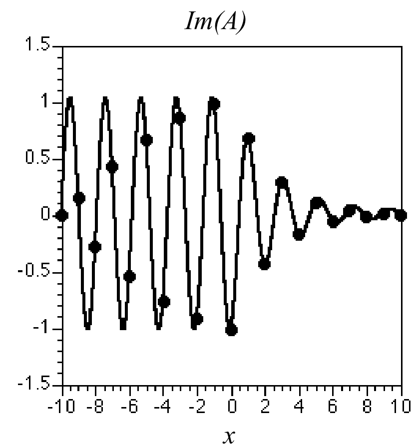

Figure 3: 1D heterogeneous problem, the imaginary part of the solution. Heterogeneous domain with -10 ≤ x ≤ 10 in normalized length scales. For x ≤ 0, k = 3, while for x ≥ 0, k = 3 + 0.4i. The solid line represents the exact analytical solution. The dots represent the random-walk solution points.

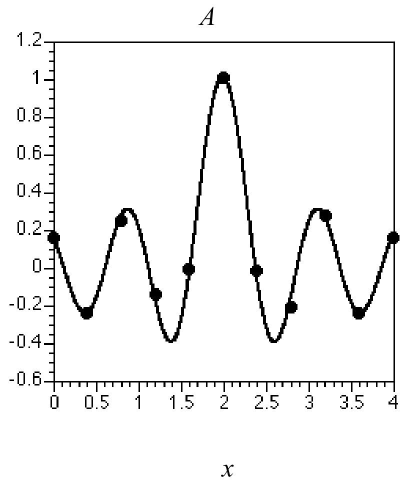

Figure 4: 2D homogeneous problem in an insulating circular cross section of diameter 4λ in normalized length scales with k = 1. A solution consisting of the zeroth order Bessel function is imposed. The solution is plotted along a diameter of the cross section. The solid line represents the exact analytical solution. The dots represent the random-walk solution points.

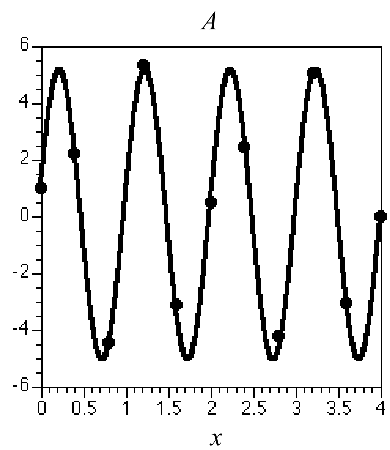

Figure 5: 2D homogeneous problem in an insulating square problem domain with a side equal to 4λ in normalized length scales and k = 1. A Fourier mode solution is imposed and the solution is plotted along the centerline x axis. The solid line represents the exact analytical solution. The dots represent the random-walk solution points.

Table 1: Computational details for the verification problems.

Problem Specifications	RWs per solution point	Time per solution point	Mean absolute error
1D Helmholtz equation with source term	20000	About 1 second	0.004 on a solution range (−0.8 to 0.8)
1D Helmholtz equation in heterogeneous problem domain	500	About 1 second	$(1.7+2.8i)\times10^{-15}$ on a solution range $(-1-i)$ to $(1+i)$
2D Helmholtz equation with a zeroth order Bessel function solution	15000	About 1 minute	$0.027+0.017i$ on a solution range (−0.4 to +1.0)
2D Helmholtz equation with a Fourier mode solution	15000	About one minute	$0.106+0.143i$ on a solution range (−5 to +5)

4. Conclusions

In conclusion, we have been able to create a floating RW algorithm for Maxwell-Helmholtz equations at multiple wavelength scales. Our next goal is to extend this approach to heterogeneous problems in 2D and 3D. The absence of analytical Green's function in 2D and 3D for structures of arbitrary heterogeneity makes this an interesting problem. A possible future application of this algorithm would be the extraction of frequency- dependent inductance, resistance and capacitance. We believe that with additional development, this algorithm will lead to the development of IC CAD for high-end digital IC interconnect systems.

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