A Monte Carlo Algorithm for the Solution of the One-Dimensional Wave Equation

K. CHATTERJEE[α], C. YU
Department of Electrical and Computer Engineering
The Cooper Union
51 Astor Place, New York, NY 10003-7185
THE UNITED STATES OF AMERICA

Abstract: - This paper presents a 1D Monte Carlo (MC) algorithm for the solution of the wave equation. Historically, the MC method has not been applied successfully to the solution of wave problems. This can primarily be attributed to the problem of resonance in the frequency-domain Green's function for finite geometries at length scales greater than half a wavelength. In our previously published work, we have been successful in obtaining a frequency-domain solution at multiple-wavelength length scales through the use of infinite-domain Green's functions. In this work, we extend the algorithm to problems in the time-domain. The MC method does not require any discretization, and hence the memory requirements are lower than approaches based on discretization. Another advantage of the MC method is that the computational procedure is inherently parallelizable and an almost linear increase in computational speed can be obtained with an increase in the number of processors. The application area of our interest is in the full-wave analysis of IC interconnect structures at multi-GHz frequencies.

Key-Words: - Monte Carlo, Wave equation, IC interconnect analysis

1 Introduction

The solution of the wave equation has widespread applications in science and engineering. Our particular area of interest is in the electromagnetic analysis of IC interconnect structures, where recent advances have resulted in multi-GHz operating frequencies. At such frequencies, circuit designers must account for a number of electromagnetic effects that are difficult to estimate. These effects include skin-effect loss, frequency-dependent inductance and capacitance, slow-wave substrate coupling, distributed transmission-line propagation and high-frequency radiation. With increasing frequencies, it is becoming evident that the electrical properties of IC interconnects must be estimated through a direct solution of Maxwell's equations. However, traditional methods for the numerical solution of Maxwell's equations require discretization both in space and time and the resulting computational difficulty becomes somewhat unmanageable in complicated 3D problem domains. As a result, we have been in the process of developing a MC [1-3] methodology for the solution of Maxwell's equations. The MC method is based on probabilistic interpretations of deterministic equations. The method is completely meshless and hence the memory requirements for complicated problem geometries are significantly lower than for methods based on spatial discretization. Furthermore, the method is inherently parallelizable and an almost linear increase in speed can be obtained with an increase in the number of processors [4]. However, in spite of all these advantages, stochastic solution methodologies for hyperbolic PDEs are hard to formulate. This difficulty can primarily be attributed to the fact that there is a fundamental link between diffusion and Brownian motion [5], while hyperbolic problems model propagation without distortion. The mathematical foundations of a stochastic model of the wave equation have been laid out by Mark Kac and Sidney Goldstein [6]. However, there is an absence of effective MC algorithms for the wave equation. This is due to the problem of resonance in the frequency-domain Green's function [7-8] at multiples of half-a-wavelength length scales, which will be described in the next section.

Our previous work [9] has involved the development of a MC algorithm for Maxwell's equation (in the frequency domain) through an iterative-perturbation based Green's function in problem domains of arbitrary heterogeneity and thus

[α] Adjunct Scientist at the Laboratory for Electromagnetic and Electronic Systems, Massachusetts Institute of Technology, Cambridge, MA 02139-4307, USA

very suited for materially heterogeneous interconnect structures. Though this algorithm was able to capture quasi-static effects such as skin-effect, it was limited to length scales smaller than half a wavelength. In a later work [10-11], we were able to extend the frequency-domain solution to multiple-wavelength length scales through the use of an infinite-domain Green's function. In this present work, we develop a MC algorithm for the 1D wave equation in the time-domain. We will now present the details of the algorithm.

2 Development of the Algorithm

We consider the 1D wave equation

$$\frac{\partial^2 U}{\partial t^2} = v^2 \frac{\partial^2 U}{\partial x^2}, \tag{1}$$

defined in domain $0 \le x \le L$, v being the speed of propagation. The speed of propagation is assumed to be equal to unity ($v = 1\,m/s$) everywhere in this paper. We impose the following initial and boundary conditions,

$$\begin{aligned} &U(0,t) = 0,\ U(L,t) = 1, \\ &U(x,0) = \sin\left(\frac{c\pi x}{L}\right) + \frac{x}{L}, \\ &\frac{\partial U}{\partial t}(x,0) = \frac{d\pi}{L}\sin\left(\frac{d\pi x}{L}\right), \end{aligned} \tag{2}$$

where c and d are integers. With the method of eigenfunction expansion [7-8], the analytical solution Eq. (1) can be shown to be

$$\begin{aligned} U(x,t) &= \cos\left(\frac{c\pi t}{L}\right)\sin\left(\frac{c\pi x}{L}\right) \\ &+ \sin\left(\frac{d\pi t}{L}\right)\sin\left(\frac{d\pi x}{L}\right) + \frac{x}{L}. \end{aligned} \tag{3}$$

We now consider a Green's function [7-8] $G(x,t \mid x_0,t_0)$, to Eq. (1) whose solution at (x,t) is given as the solution of the equation

$$\frac{\partial^2 G}{\partial t^2} - \frac{\partial^2 G}{\partial x^2} = \delta(x - x_0)\delta(t - t_0), \tag{4}$$

given a dirac-delta function source at (x_0,t_0) subject to the following homogeneous boundary conditions and causal initial conditions:

$$\begin{aligned} &G(0,x_0 \mid t,t_0) = G(L,x_0 \mid t,t_0) = 0, \\ &\left[G(x,t \mid x_0,t_0)\right]_{=t_0^-} = 0, \\ &\left[\frac{\partial G}{\partial t}(x,t \mid x_0,t_0)\right]_{t=t_o^-} = 0. \end{aligned} \tag{5}$$

Again, using the method of eigenfunction expansion [7-8], the Green's function can be shown to be

$$\begin{aligned} G(x,t \mid x_0,t_0) &= \sum_{n=1}^{\infty} \frac{2}{\pi n}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x_0}{L}\right) \\ &\times \sin\left(\frac{n\pi}{L}(t - t_0)\right)H(t - t_0), \end{aligned} \tag{6}$$

where $H(t - t_0)$ is the unit-step [7-8] function. Using Green's integral theorem, the solution at any point x inside the problem domain $[0,L]$ at time t is given by

$$\begin{aligned} U(x,t) &= \int_{x_0=0}^{x_0=L}\left[\frac{\partial U}{\partial t_0}(x_0,0)G(x,t \mid x_0,0)\right]dx_0 \\ &- \int_{x_0=0}^{x_0=L}\left[U(x_0,0)\frac{\partial G}{\partial t_0}(x,t \mid x_0,0)\right]dx_0 \\ &- \int_{t_o=0}^{t_o=t}\left[U(L,t_0)\frac{\partial G}{\partial x_0}(x,t \mid L,t_0)\right]dt_0 \\ &+ \int_{t_o=0}^{t_o=t}\left[U(0,t_0)\frac{\partial G}{\partial x_0}(x,t \mid 0,t_0)\right]dt_0 \end{aligned} \tag{7}$$

We now introduce a new variable $S(x,t)$, such that $S(x,t) = U(x,t) - \frac{x}{L}$. Hence, Eq. (7) transforms to

$$S(x,t) = \int_{x_0=0}^{x_0=L} \left[\frac{\partial S}{\partial t_0}(x_0,0) G(x,t \mid x_0,0) \right] dx_0$$
$$- \int_{x_0=0}^{x_0=L} \left[S(x_0,0) \frac{\partial G}{\partial t_0}(x,t \mid x_0,0) \right] dx_0, \quad (8)$$
$$U(x,t) = S(x,t) + \frac{x}{L}.$$

Hence, the MC solution of the boundary-value problem given in Eq. (1) reduces to the statistical estimation [12] of the two line integrals in Eq. (8), which is achieved by sampling the integrand with the help of a random-number generator, according to a pre-determined probability distribution function. The two line integrals in Eq. (8) readily generalize to surface and volume integrals for problems in two and three dimensions [7-8]. An estimate of the solution, $\overline{U}(x,t)$ is obtained by averaging over a statistically large number (N) of samples of the variable $S(x,t)$, and is given by

$$\overline{S} = \frac{1}{N} \sum_{n=1}^{N} S_n,$$
$$\overline{U} = \overline{S} + \frac{x}{L}. \quad (9)$$

where S_n is the nth sample, and $\overline{S}$ and $\overline{U}$ are statistical estimates of $S(x,t)$ and $U(x,t)$. Thus the solution $U(x,t)$ at a given position and time can be estimated irrespective of the solution at any other position or time.

There are two kinds of error in this algorithm. The first source of error stems from the truncation of the Green's function in Eq. (6) and its temporal derivative as used in Eq. (8). The second source of error in the result is statistical in nature. A measure σ_T of the statistical error is given by [13]

$$\sigma_T = \frac{\sigma_E}{\sqrt{N}}, \quad (10)$$

where σ_E is the standard deviation of the estimates from different integration samples of the variable $S(x,t)$, and N is the number of samples. As a result, the statistical error can be controlled by controlling the number of samples.

We note that the form of the Green's function in Eq. (6) does not impose any restriction on the length of the problem domain L. On the other hand, the Green's function equation to Eq. (1) in the frequency domain is given by

$$\frac{\partial^2 G(x \mid x_0)}{\partial x^2} + \omega^2 G(x \mid x_0) = \delta(x - x_0), \quad (11)$$

where ω is the frequency, with boundary conditions $G(0 \mid x_0) = 0$ and $G(L \mid x_0) = 0$. The solution to Eq. (11) is given by [7-8]

$$G(x \mid x_0) = \frac{\sin[\omega(x_0 - L)]}{\omega \sin(\omega L)} \sin(\omega x), \quad x < x_0,$$
$$G(x \mid x_0) = \frac{\sin(\omega x_0)}{\omega \sin(\omega L)} \sin[\omega(x - L)], \; x > x_0. \quad (12)$$

It can be seen that for $\omega L = n\pi$, (n being an integer), $\sin(\omega L) = 0$, and it is not possible to achieve a statistical solution beyond half a wavelength length scales. As a consequence of this resonance in the frequency-domain, the MC method has not been widely applied to the solution of the wave equation. In a previous work [10-11], we were able to achieve a stochastic solution at multiple wavelengths through the use of an infinite-domain Green's function of the form:

$$G(x \mid x_0) = \frac{1}{2\omega} \sin(\omega |x - x_0|) \quad (13)$$

In this work, we have developed a MC algorithm for problems in the time-domain. The results are given in the next section.

3 Results

We have applied the MC algorithm to two benchmark problems:

$$U(0,t)=0,\ U(L,t)=1,$$
$$U(x,0)=\sin\left(\frac{c\pi x}{L}\right)+\frac{x}{L},\ c=4, \qquad \text{(A)}$$
$$\frac{\partial U}{\partial t}(x,0)=0.$$

and

$$U(0,t)=0,\ U(L,t)=1,$$
$$U(x,0)=0, \qquad \text{(B)}$$
$$\frac{\partial U}{\partial t}(x,0)=\frac{d\pi}{L}\sin\left(\frac{d\pi x}{L}\right),\ d=5.$$

As mentioned in the previous section, the speed of propagation is assumed to be equal to $1 m/s$ and the problems are simulated for $L=4\pi$ meters and $t=1$ second. The algorithm was coded in C on a 2 GHz Apple MacBook and 10^6 random-walks were generated for each solution point. The Green's function in Eq. (6) and its temporal derivative in Eq. (8) were truncated to 250 terms. It can be observed from Fig. 1 and Fig. 2, that there is excellent agreement between analytical and MC solutions. Table 1 shows the exact and statistical error (given by Eq. 10), and they are seen to be in conformity.

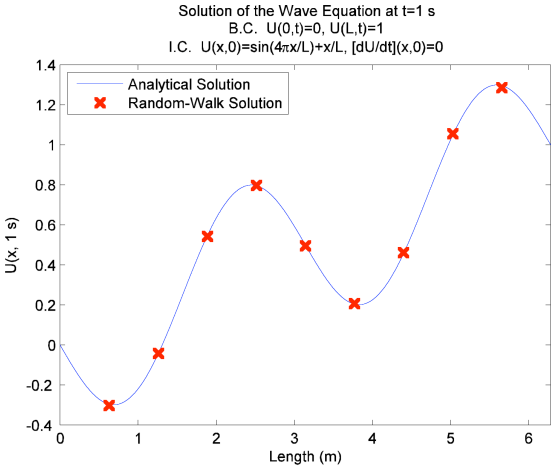

Fig. 1: Solution of the wave equation in Eq. (1) with $L=4\pi$ meters and $t=1$ second for the initial and boundary conditions shown above. The speed of propagation is assumed to be unity (i.e. $1\ m/s$).

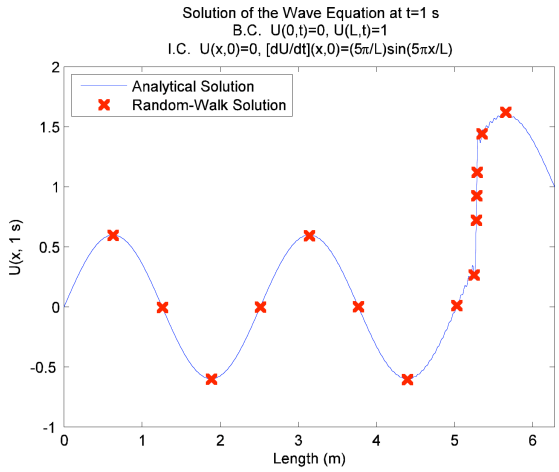

Fig. 2: Solution of the wave equation in Eq. (1) with $L=4\pi$ meters and $t=1$ second for the initial and boundary conditions shown above. The speed of propagation is assumed to be unity (i.e. $1\ m/s$).

Problem Specification	Exact Error	Statistical Error
Problem A	0.004	0.006
Problem B	0.002	0.002

Table 1: Exact and statistical errors for the benchmark problems. The errors are normalized to the maximum value of the solution in each case.

4 Conclusion and Future Work

Summarizing, we have developed a 1D MC algorithm for the wave equation and excellent agreement has been obtained between our numerical results and exact analytical solutions. We plan to extend the algorithm to problems in materially heterogeneous problem domains, to problems in two and three dimensions, as well as to Neumann and mixed boundary condition problems. We also plan to collaborate with researchers at Air Force Research Laboratory (Wright-Patterson Air Force Base) towards achieving the parallelization and optimization of this algorithm.

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