The application of recursive aggregate T-matrix algorithm in the Monte Carlo simulations of the extinction rate of random distribution of particles

C. C. Lu and W. C. Chew

Department of Electrical and Computer Engineering, University of Illinois, Urbana

L. Tsang

Department of Electrical Engineering, University of Washington, Seattle

Abstract. The recursive T -matrix algorithm is applied to Monte Carlo simulations of multiple scattering by random distribution of dielectric spheres. The method is a fast algorithm for calculating the exact solution of Maxwell's equations for a large number of scattering objects. The extinction rate is calculated by averaging over many realizations. The computed results are compared with those from analytic approximations, namely, the quasi-crystalline approximation.

Introduction

Investigation of the scattering properties of randomly distributed particles has applications in wave propagation and remote sensing [*Tsang et al.*, 1985; *Tsang and Kong*, 1980]. The classical approximation was based on the independent scattering assumption, i.e., the coherent wave interactions between particles are ignored. For example, based on the independent approximation, the extinction rate is linearly proportional to the concentration or fractional volume of particles. This is not true when the density of the particles is increased. Later on, there are approximate analytical solutions, e.g., Foldy's approximation, bilocal approximation, quasi-crystalline approximation, and quasi-crystalline approximation with coherent potential (QCA-CP), which take into account the coherent multiple-scattering effects [*Tsang et al.*, 1985; *Tsang and Kong*, 1980]. To take into account correlated scattering, the pair distribution functions also have to be used. A common approximation is to make use of the Percus-Yevick (PY) approximation. Many of these analytic approximations are difficult to justify. Thus with the advent of modern computers, it is important to solve Maxwell's equation exactly for media involving a large number of particles and to compare the results with those from analytic approximations. By using the T -matrix, Maxwell's equations are converted into Foldy Lax multiple-scattering equations [*Tsang et al.*, 1985]. Translational addition theorems are used to transform spherical waves from one center of a sphere to another sphere. The equations are exact without approximations and include coherent mutual interaction of waves among scatterers. Based on this set of equations, numerical simulation was done recently by *Tsang et al.* [1992], using a direct iterative method.

Such simulations of random media electromagnetic scattering are large-scale problems, because beside the large number of scatterers that have to be included in the geometrical configuration, the multiple-scattering equations have to be solved for many realizations, and the average scattering is then calculated. Thus it is important to develop an efficient computation algorithm [*Chew*, 1990; *Chew and Wang*, 1990, 1993; *Chew and Lu*, 1993; *Wang and Chew*, 1993]. We present a simulation with a different method for solving the scattering properties. The scattering solution method is the Recursive Aggregate T-Matrix Algorithm (RATMA) [*Chew*, 1990; *Chew and Wang,* 1990], which is very efficient in solving the scattering problem by a large number of spheres. This method has two major advantages: one is the reduction in computational complexity, and the other is the reduction in memory requirement. The computed results are compared with independent scattering and quasi-crystalline approximation with coherent potential and Percus-Yevick approximation (QCA-CP-PY) [*Tsang and Kong*, 1980].

Formulation

Consider an incident electromagnetic wave with incident wave vector $\mathbf{k}_i$ scattered by a medium consisting of N spheres centered at $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$ with radii equal to a and with permittivities ϵ_s. The background medium has permittivity ϵ. The particles are embedded in a volume V. The solution of Maxwell's equations including all multiple scattering can be cast into the following matrix equation [*Tsang et al.*, 1985; *Chew*, 1990]:

$$\mathbf{w}^{(\alpha)} = \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N} \overline{\boldsymbol{\sigma}}(k, \mathbf{r}_\alpha, \mathbf{r}_\beta) \cdot \overline{\mathbf{T}}_1^{(\beta)} \cdot \mathbf{w}^{(\beta)} + e^{i\mathbf{k}_i\cdot\mathbf{r}_\alpha}\mathbf{a}_{inc} \tag{1}$$

with $\alpha = 1, 2, \ldots, N$, where we have used the notation of *Tsang et al.* [1985]. In (1), $\mathbf{w}^{(\alpha)}$ is a column matrix representing the exciting field of the scatterer α, i.e., the "final" field exciting scatterer α including multiple-scattering effects; $\mathbf{a}_{inc}$ is a column matrix containing the coefficients of the incident wave, $\overline{\mathbf{T}}_1^{(\beta)}$ is the T -matrix representing scattering from the scatterer β, and the subscript 1 denotes that it is a single-particle T -matrix. In (1), $\overline{\boldsymbol{\sigma}}(k, \mathbf{r}_\alpha, \mathbf{r}_\beta)$ is a vector spherical wave transformation matrix that translates spherical waves of multipole fields centered at $\mathbf{r}_\beta$ to multipole spherical waves centered at $\mathbf{r}_\alpha$. The physical interpretation of (1) is that the field-exciting scatterer α is the sum of the incident field and the scattered field from all other particles except itself. Thus equation (1) contains multiple-scattering effects. The result includes near-field, intermediate, and far-field interactions because $\overline{\boldsymbol{\sigma}}$ is an exact wave transformation.

The multiply scattered field $\mathbf{a}^{s(\alpha)}$ of particle α is

$$\mathbf{a}^{s(\alpha)} = \overline{\mathbf{T}}_1^{(\alpha)} \cdot \mathbf{w}^{(\alpha)} \tag{2}$$

In (1) and (2), $\overline{\mathbf{T}}_1^{(\alpha)}$ is the T -matrix solution of a single sphere. In the RATMA algorithm of solving (1), an N -particle aggregate T matrix is defined so that

$$\mathbf{a}^{s(\alpha)} = \overline{\boldsymbol{\tau}}_{(N)} \cdot \exp{(i\mathbf{k}_i \cdot \mathbf{r}_0)}\mathbf{a}_{inc} \tag{3}$$

where $\overline{\boldsymbol{\tau}}_{(N)}$ is the aggregate T -matrix of the N particles present in the configuration. Note that the last term in (3) is $\mathbf{a}_{inc}$, the incident field, rather than $\mathbf{w}^{(\alpha)}$, the exciting field, as in equation (2).

In RATMA, one first calculates $\overline{\mathbf{T}}_1^{(\alpha)}$, which is the Mie solution for one particle. At the $(n{+}1)$th step, the n sphere solution of $\overline{\boldsymbol{\tau}}_{(n)}$ is used to construct the $n+1$ sphere solution of $\overline{\boldsymbol{\tau}}_{(n+1)}$. This method takes into account all the interactions between spheres. This is repeated recursively until $\overline{\boldsymbol{\tau}}_{(N)}$ is obtained. It is interesting to note that the aggregate T -matrix can be used to calculate the scattered field for arbitrary incident waves, though only one incident direction is used in this simulation. An efficient method has also been devised to calculate the $\overline{\boldsymbol{\sigma}}$ from the vector translational addition theorem [*Chew and Wang*, 1993].

In random media scattering problems, the scattered field can be decomposed into the coherent field $\langle \mathbf{E}_s \rangle$ and incoherent field $\boldsymbol{\varepsilon}_s$. In the numerical simulations, the coherent scattered field

$\langle \mathbf{E}_s \rangle$ is calculated by

$$\langle \mathbf{E}_s \rangle = \frac{R}{N_r} \sum_{\sigma=1}^{N_r} \mathbf{E}_s^\sigma \tag{4}$$

and the incoherent scattered field is $\boldsymbol{\varepsilon}_s^\sigma = \mathbf{E}_s^\sigma - \langle \mathbf{E}_s \rangle$, where σ is the realization index with $\sigma = 1, 2, \ldots, N_r$ realizations. The coherent scattered field is peaked in the forward direction and becomes an angular Dirac delta function in the forward direction in the idealized situation of infinite volume V and infinite number N. For finite but large V, the coherent forward scattered field is many decibels higher than other directions. However, coherent forward scattering is not to be counted as extinction. The extinction arises from the incoherent scattered field. Thus the average bistatic scattering cross section of the N particle ensemble is

$$\sigma_{bN}(\hat{k}_s, \hat{k}_i) = R^2 \langle |\boldsymbol{\varepsilon}_s^\sigma|^2 \rangle = \frac{R^2}{N_r} \sum_{\sigma=1}^{N_r} |\boldsymbol{\varepsilon}_s^\sigma|^2 \tag{5}$$

The average scattering cross section of N particles is the integration of (5) over scattering angles. The coherent wave attenuation rate κ_e is the extinction cross section per unit volume,

$$\kappa_e = \lim_{V \to large} \frac{1}{V} \int_0^\pi d\theta_s \sin\theta_s \int_0^{2\pi} d\phi_s \sigma_{bN}, \tag{6}$$

where, σ_{bN} is a function of $(\hat{k}_s, \hat{k}_i)$.

Numerical Results

Using the program that generates the random positions of particles for a medium consisting of dense distribution of particles [*Ding et al.*, 1992], we first generate a cluster of randomly distributed spheres which occupies a cubic volume. In the random positioning of particles, the particles do not exert mutual force among themselves. However, they are not allowed to interpenetrate. Such noninterpenetration criteria lead to nontrivial pair distribution functions such as the Percus-Yevick type for densely packed spheres [*Tsang et al.*, 1985; *Wang and Chew*, 1993]. To be more practical, only the spheres that are in a spherical volume are selected (the spherical volume is contained in the cubic box).

In order to compare the result, the parameters of simulation used in this paper are selected to be the same as those used by [*Tsang et al.* 1992], i.e., $ka = 0.2, \epsilon_r = 3.2$ with fractional volume varying from 0.05 to 0.20. Figure 1 shows the normalized extinction rate as a function of fractional volume using 500 spheres and 20 realizations. The result is close to that of the approximate theory of QCA-CP-PY and departs significantly from the linear curve of independent scattering. Figure 2 shows the convergence as a function of realizations. Because of angular integration to calculate the extinction, only 20–30 realizations are required to achieve convergence. It is seen that there is a small difference in the two polarizations; this difference is partly due to the inhomogeneity of the objects. We have considered using the rotated objects as different realizations in order to fully utilize the T -matrix results. The computed extinction rate in this way is smaller than that using totally physical realization. One explanation is that the correlation between rotated objects is larger than that between different realizations. In Figure 3, the results are calculated based on 2000 dielectric spheres. Comparing the results of Figures 1 and 3 shows the convergence with respect to the number of spheres used.

Conclusion

The RATMA algorithm is used to compute the scattered field in the Monte Carlo simulations. The numerical result is in agreement with previous results up to 25% by volume. This method needs smaller memory and can be easily used to deal with a larger number of particles. We are presently extending the algorithm to handle larger-scale problems for larger particle sizes and higher densities than 25% by volume [*Chew and Lu*, 1993].

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W. C. Chew and C. C. Lu, Department of Electrical and Computer Engineering, University of Illinois, Urbana, IL 61801. (e-mail: caicheng@bspark.ece.uiuc.edu and w-chew@uiuc.edu)

L. Tsang, Department of Electrical Engineering, FT-10, University of Washington, Seattle, WA 98195. (e-mail: tsang1@max.u.washington.edu)

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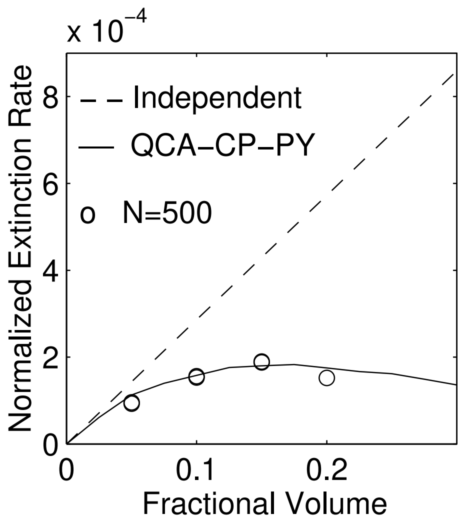

Figure 1.

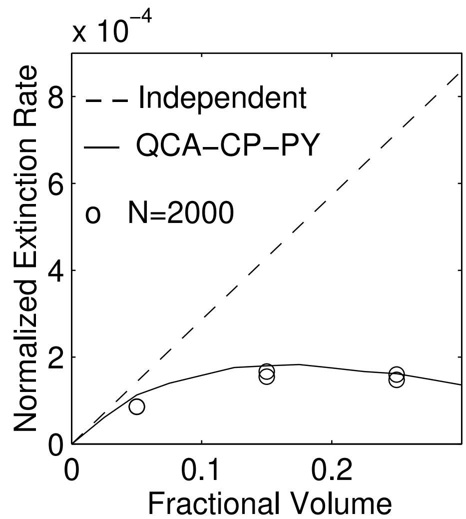

Figure 3.

Figure 1. Normalized extinction rate as a function of fractional volume.

Figure 3. Combined result of realizations and rotations.

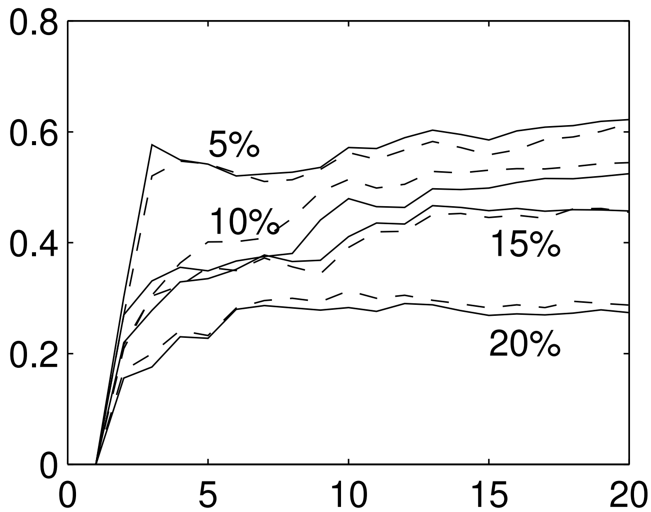

Figure 2. Convergence curve (fractional volume as parameters).