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Pseudospectral time domain simulations of multiple light scattering in three-dimensional macroscopic random media

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[1] We report a full-vector, three-dimensional, numerical solution of Maxwell's equations for optical propagation within, and scattering by, a random medium of macroscopic dimensions. The total scattering cross section is determined using the pseudospectral time domain technique. Specific results reported in this paper indicate that multiply scattered light also contains information that can be extracted by the proposed cross-correlation analysis. On a broader perspective, our results demonstrate the feasibility of accurately determining the optical characteristics of arbitrary, macroscopic random media, including geometries with continuous variations of refractive index. Specifically, our results point toward the new possibilities of tissue optics; by numerically solving Maxwell's equations, the optical properties of tissue structures can be determined unambiguously.

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1. Introduction

[2] Light scattering by macroscopic, low-contrast random media, such as biological tissue structures, is generally a very difficult problem to study analytically because of the enormous number of variables involved. Nevertheless, it continues to be studied in various disciplines [*Barrowes et al.*, 2000, *Jaruwatanadilok et al.*, 2003, *Mishchenko et al.*, 2004] with a common challenge: the analysis of scattered electromagnetic waves to acquire geometrical information about the random media.

[3] Conventionally, various degrees of heuristic approximations are employed to simplify the problem, including Monte Carlo technique [*Welch and van Gemert*, 1995], the effective medium theory [*Busch and Soukoulis*, 1995], and approximation methods based on radiative transfer theory, such as Beer's Law, Kubelka-Monk approximations, the adding-doubling method, the diffusion approximation. These methods, however, generally neglect the full-vector electromagnetic wave nature of light, such as the near-field interactions and coherent interference effects, resulting in questionable accuracy and validity [*Marti-Lopez et al.*, 2003]. In order to properly characterize optical properties of closely packed scatterers, a rigorous method based on fundamental electromagnetic theory is desired.

2. Pseudospectral Time Domain (PSTD) Simulations

[4] In this paper, we report the initial application to the tissue optics problem of an emerging advanced variant of the finite difference time domain (FDTD) technique: the pseudospectral time domain (PSTD) technique [*Liu*, 1997]. For large electromagnetic wave interaction models in D dimensions not having geometric details or material inhomogeneities smaller than one-half wavelength, PSTD reduces computer storage and running time by approximately $4^D \sim 8^D$, relative to standard FDTD while achieving comparable accuracy [*Liu*, 1999]. This advantage is sufficient to permit rigorous numerical solution of the full-vector Maxwell's equations for optical propagation within, and scattering by, a random medium of macroscopic dimensions.

[5] The most basic version of PSTD is implemented on an unstaggered, collocated Cartesian space grid. Let $\{V_i\}$ denote the values of field component V at all points along an x-directed cut through the grid, and let $\{(\partial V/\partial x)_i\}$

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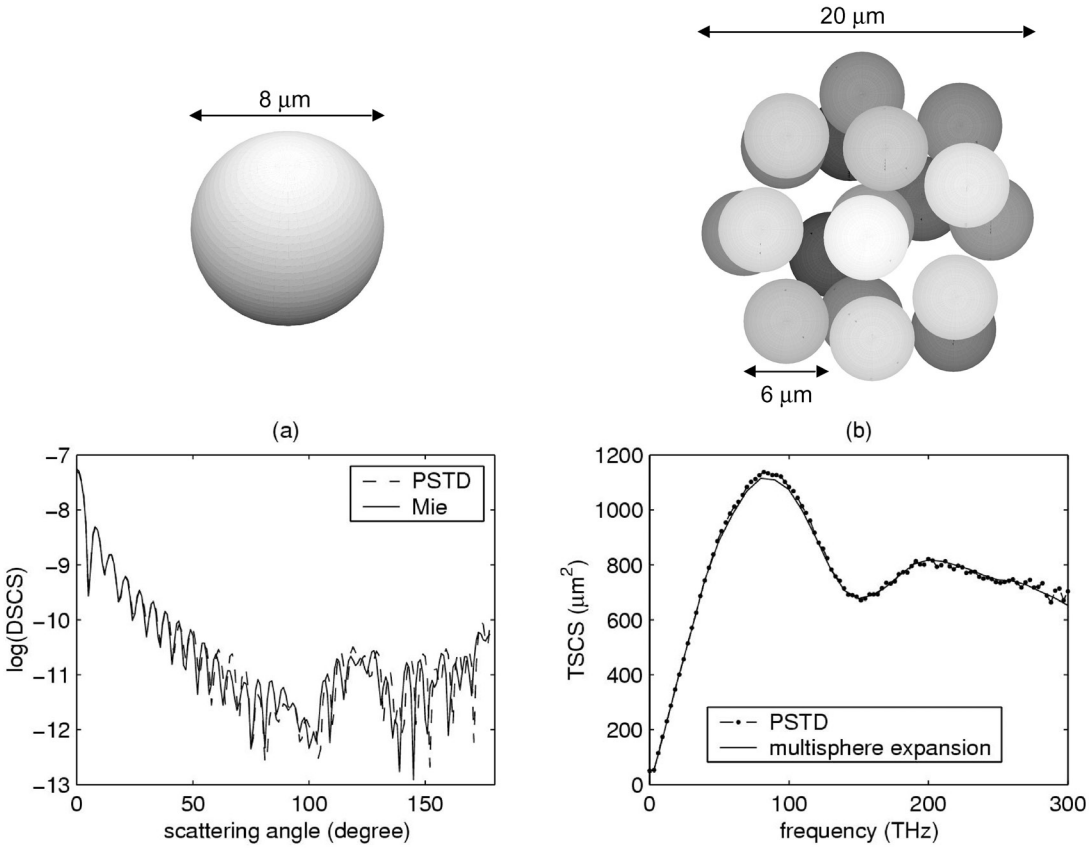

Figure 1. Validation of the 3-D PSTD simulations. (a) PSTD-computed differential scattering cross section as a function of angle is compared with the analytical solution (Mie expansion). Light scattering (wavelength $\lambda_0 = 0.75$ μm) by a single 8-μm-diameter, dielectric ($n = 1.2$) sphere is simulated using the PSTD technique, with a grid resolution of $dx = 0.0833$ μm. (b) PSTD-computed TSCS as a function of frequency is compared with the multisphere expansion. Light scattering (wavelength $\lambda_0 = 1$ μm) by a 20-μm-diameter cluster consisting of 19 randomly positioned, 6-μm-diameter, dielectric spheres is simulated using the PSTD technique, with a grid resolution of $dx = 0.167$ μm.

denote the x derivatives of V at the same points needed in Maxwell's equations. Using the differentiation theorem for Fourier transforms, we can write

$$\left\{\left.\frac{\partial V}{\partial x}\right|_i\right\} = -\mathbf{F}^{-1}\left(j\tilde{k}_x \mathbf{F}\{V_i\}\right) \tag{1}$$

where $\mathbf{F}$ and $\mathbf{F}^{-1}$ denote, respectively, the forward and inverse discrete Fourier transforms, and $\tilde{k}_x$ is the Fourier transform variable representing the x component of the numerical wave vector. In this way, $\{(\partial V/\partial x)_i\}$ can be calculated in one step. In multiple dimensions, this process is repeated for each cut parallel to the major axes of the space lattice.

[6] According to the Nyquist sampling theorem, the representation in (1) is exact (i.e., of "spectral accuracy") for electromagnetic field spatial modes sampled at the Nyquist rate or better. This permits the PSTD meshing density to approach two samples per wavelength in each spatial dimension. The wraparound caused by the periodicity in the discrete Fourier transform is eliminated by using the anisotropic perfectly matched layer absorbing boundary condition [*Gedney*, 1996].

[7] For electromagnetic wave interaction, PSTD has been shown to exhibit the same computational accuracy and dynamic range as FDTD models having approximately eight times finer resolution [*Liu*, 1999]. That is, a PSTD grid with coarse $\lambda_d/4$ resolution provides about the same accuracy as an FDTD grid with fine $\lambda_d/32$ resolu-

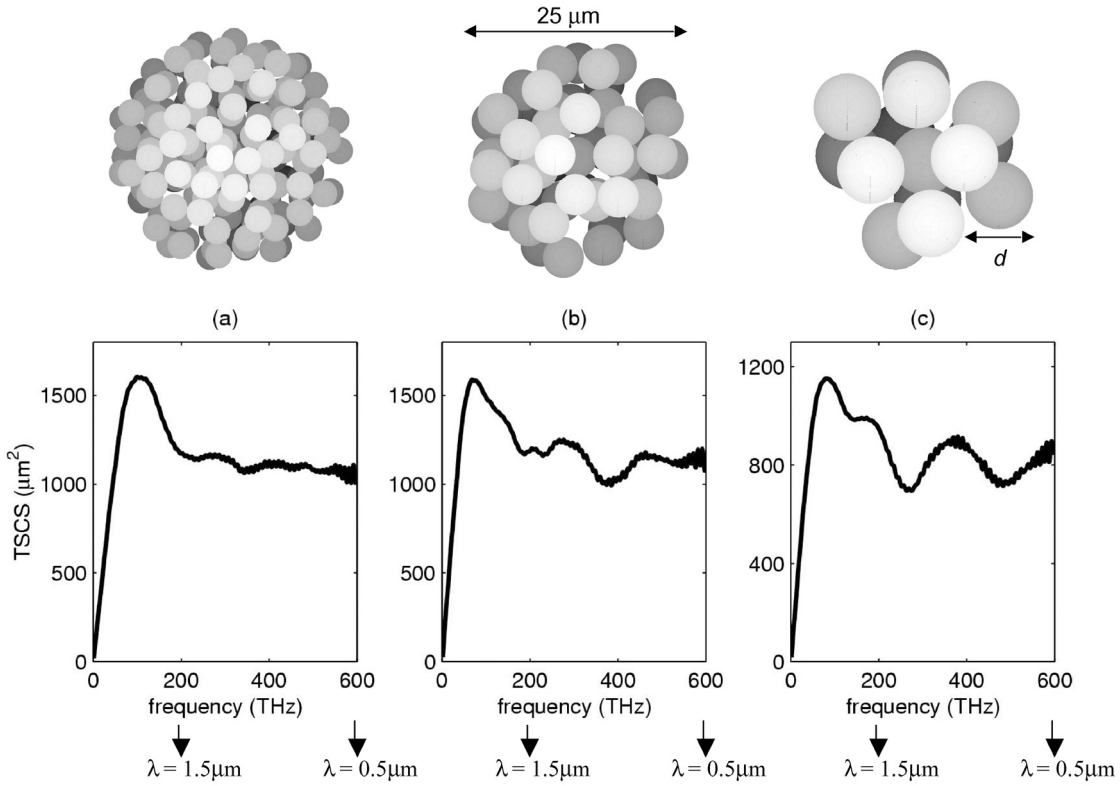

Figure 2. PSTD-computed TSCS spectra of 25-μm-diameter clusters consisting of N randomly positioned, closely packed, homogeneous, dielectric (n = 1.2) spheres of diameter d. With a PSTD grid resolution of 0.167 μm, three cases are shown: (a) d = 3 μm and N = 192, with an optical thickness ~26; (b) d = 5 μm and N = 56, with an optical thickness ~21; (c) d = 7 μm and N = 14, with an optical thickness ~10 (optical thickness is equal to geometrical thickness divided by scattering mean free path).

tion. Much experience with FDTD modeling has shown that this level of spatial resolution yields accuracy of better than 1 dB over dynamic ranges exceeding 50 dB for the scattering intensity observed at all possible angles.

3. Results and Analysis

[8] In this paper, we report application of PSTD technique to model full-vector, three-dimensional (3-D) scattering of light by macroscopic clusters of dielectric spheres in free space. We use a PSTD grid having a uniform spatial resolution of 0.167 μm, equivalent to $0.33\lambda_d$ at 600 THz (λ_0 = 0.5 μm) for a refractive index n = 1.2.

[9] Validation of our research methodology is shown in Figure 1, where the light scattering properties of: (1) a homogeneous dielectric sphere, (2) a cluster of N = 19 randomly positioned, dielectric spheres, are calculated using PSTD simulations and compared with the analytical solution: Mie expansion [*Mie*, 1908] and multisphere expansion [*Xu and Wang*, 1998], respectively. Even with a coarse resolution (three grid points per wavelength), PSTD simulation yields excellent agreement with the analytical expansions. Nevertheless, the primary drawback is that the sample geometry is resolved only to the extent determined by the grid resolution.

[10] The dielectric spheres were positioned randomly with a minimum (edge-to-edge) spacing of 0.25 μm between spheres. A standard anisotropic perfectly matched layer (APML) absorbing boundary condition [*Gedney*, 1996] is implemented to absorb outgoing waves, simulating an open-region light-scattering experiment. An impulsive plane wave illuminates the cluster, allowing scattered light of various wavelengths at all angles to be obtained in a single run by employing a near-to-far field transformation [*Taflove and Hagness*, 2000].

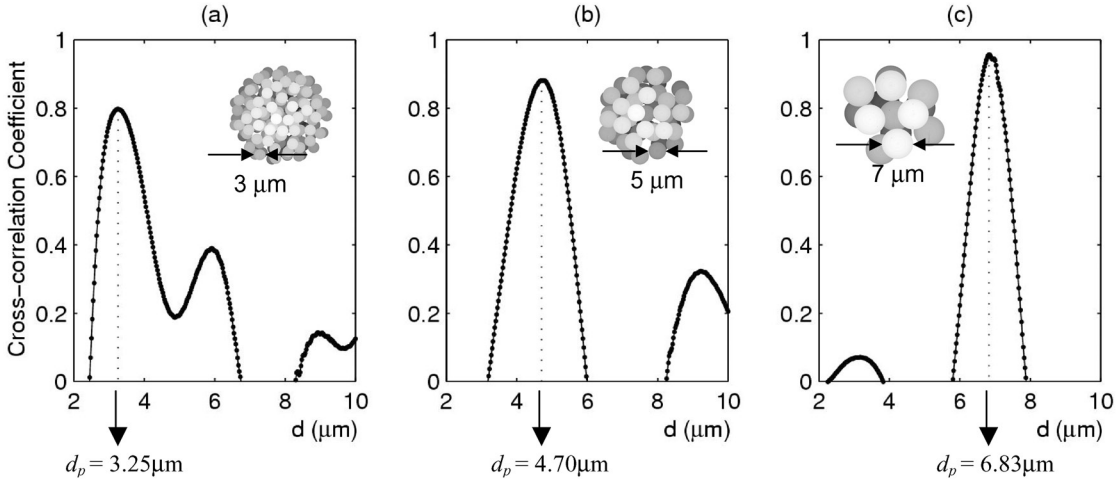

Figure 3. Cross-correlation analysis of the TSCS spectra shown in Figure 2. By calculating the cross-correlation coefficients of the cluster TSCS (as shown in Figures 2a–2c) and the TSCS spectra of a single dielectric sphere, it is shown that the correlation coefficient peaks at $d = d_p$, where d_p is approximately equal to the diameter of the constituent spheres of the cluster geometry.

[11] By employing the PSTD algorithm, light scattering by a cluster of closely packed dielectric spheres in free space is simulated, yielding the total scattering cross-section (TSCS) spectra as function of frequency from 1 to 600 THz (λ_0 = 300–0.5 μm) with a resolution of 1.0 THz. Each cluster, with a diameter D = 25 μm, consists of N randomly positioned, closely packed, noncontacting, homogeneous, dielectric (n = 1.2) d-μm-diameter spheres. The TSCS spectra corresponding to three different cluster geometries are shown in Figures 2a–2c.

[12] Notice that all three TSCS spectra are similar in the low-frequency regime ($\lambda_0 \gg 3$ μm), suggesting that for long wavelength, the incident light cannot discern the microscopic structural difference between the three geometries [*Tseng et al.*, 2004]. However, in the shorter-wavelength regime ($\lambda_0 < 3$ μm), the TSCS spectra exhibit structural differences that can potentially yield information indicative the microscopic structures [*Tseng et al.*, 2005], even for clusters consisting of closely packed scatterers as shown in Figures 2a–2c.

[13] We propose a cross-correlation analysis to further determine the correlation of the TSCS high-frequency spectral features ($\lambda_0 < 1.5$ μm) and the corresponding cluster geometries as shown in Figure 2. By cross correlating the TSCS spectra shown in Figures 2a–2c, and the TSCS spectra of a single dielectric sphere of diameter d (d ranging from 2–10 μm), it is shown in Figure 3 that the correlation coefficient is maximized at $d = d_p$, where d_p approximately matches the actual diameter of the constituent spheres of the cluster geometry. This relationship suggests that the TSCS spectral features in the short-wavelength regime ($\lambda_0 < 1.5$ μm) is related to the size of the constituent spheres, even for optically thick (optical thickness ~ 20), closely packed cluster where the edge-to-edge spacing between adjacent spheres are less than a single wavelength (<0.5 μm).

4. Conclusions

[14] On the basis of first principles, Figures 2 and 3 show that the TSCS spectra contain information indicative of the microscopic geometrical details (i.e., size of constituent spheres), even for closely packed random media where scatterers are spaced (edge-to-edge) less than a single wavelength apart. Furthermore, by employing the proposed cross-correlation analysis, information concerning the constituent scatterer size of closely packed random media can be identified and obtained from multiply scattered light. Conventionally, singly scattered light has been utilized in sizing applications while discarding multiply scattered light [*Wax*, 2005]; the results reported in this paper suggest that multiply scattered light also contains information that can be utilized by the proposed cross-correlation analysis.

[15] The largest dimensions of random media shown in this paper is ~$(30\ \mu m)^3$ for wavelength λ_0 = 0.5 μm, with a grid resolution of dx = 0.167 μm. Each PSTD simulation of such a system typically takes ~12 hours with 20 processors (2.4-GHz Pentium 4 Xeon processors.) Nevertheless, larger systems can be simulated, but would require more computer resource. The computation required is typically proportional to ~$(Nx*Ny*Nz)/(\lambda_0)^3$, where Nx, Ny, and Nz are the number of grid points in the

x, y, and z directions, respectively, and λ_0 is the shortest wavelength simulated; therefore, for wavelength $\lambda_0 = 1.0$ μm, a system of $(60\ \mu m)^3$ with a grid resolution of $dx = 0.33$ μm can be simulated using the same amount of computational power.

[16] On a broader perspective, the results reported in this paper demonstrate the feasibility of first-principle, full-vector, 3-D simulation of light scattering by macroscopic, arbitrary random media, including media with continuous variations of refractive index. More importantly, our results point toward the new possibilities of tissue optics; by numerically solving Maxwell's equations, the optical properties of tissue structures can be determined without heuristic approximations.

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