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Fast multi-particle scattering: A hybrid solver for the Maxwell equations in microstructured materials

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ABSTRACT

A variety of problems in device and materials design require the rapid forward modeling of Maxwell's equations in complex micro-structured materials. By combining high-order accurate integral equation methods with classical multiple scattering theory, we have created an effective simulation tool for materials consisting of an isotropic background in which are dispersed a large number of micro- or nano-scale metallic or dielectric substructures.

1. Introduction

We describe in this paper a simulation method for Maxwell's equations suitable for microstructured materials consisting of separated substructures which are embedded in a homogeneous background (Fig. 1). In practice, it is often the case that the shape, permittivity and permeability of the substructures are fixed and that one seeks to optimize their placement to create a specific electromagnetic response. Each new configuration, however, requires the solution of the full Maxwell equations. If there are thousands of substructures in an electrically large region (many wavelengths in size), the calculation is generally too expensive to carry out within a design loop.

In order to accelerate such calculations, we have coupled complex geometry Maxwell solvers with multiple scattering theory. Using the hybrid solver, calculations such as the one depicted in Fig. 1 require only a few minutes on a single CPU, despite the fact that there are a million degrees of freedom needed to describe the full geometry (and there would be orders of magnitude more points needed in a finite difference or finite element discretization).

Our method, which we refer to as fast multi-particle scattering (FMPS), is based on a two step procedure. First, we enclose a representative scattering substructure, such as a single pair of gold nanorods in close proximity, within a sphere S. We then build the scattering matrix for this substructure (described below) using integral equation techniques. In a second step, the solution to the full Maxwell equations can be obtained in geometries with N substructures ($N = 200$ in Fig. 1), by solving the multiple-scattering problem where the substructures have been replaced by their scattering matrices. Not only does this reduce the number of degrees of freedom required, but we have effectively preconditioned the problem by applying the solution operator to each substructure in isolation. The linear system we solve by iteration on the multi-sphere system is, therefore, well-conditioned. Further, the fast multipole method (FMM) reduces the cost of each iteration from $O(N^2)$ to $O(N \log N)$ and is particularly efficient in this setting.

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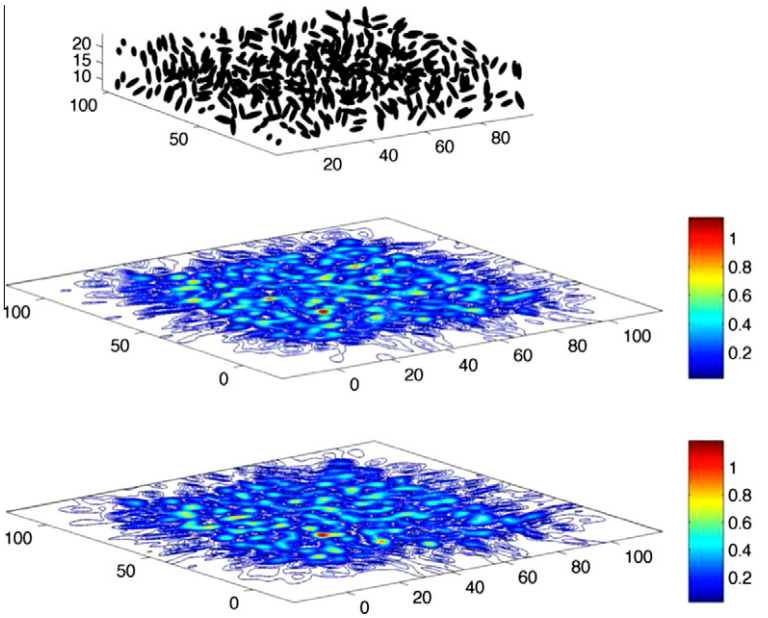

Fig. 1. Two hundred gold ellipsoid pairs are randomly oriented in the region $[0,100]\times[0,100]\times[0,20]$ and illuminated from above by a plane wave in TE polarization. The transmitted z-component of the Poynting vector is plotted on planes at $z=-4$ and $z=-8$. The individual ellipsoid pairs are of approximately unit length and the wavelength is 2π, so that the region is about $15\times15\times3$ wavelengths in size (see Section 5).

The principal limitations of the method are (1) that some modest separation distance between substructures is required and (2) that some of the efficiency is based on the fact that only a few distinct substructure types are allowed. In many experimental settings, both conditions are satisfied. We will return to a discussion of these limitations in our concluding remarks.

2. Maxwell's equations and the Debye–Lorenz–Mie formalism

Working in the frequency domain and assuming a time dependence of $e^{-i\omega t}$, Maxwell's equations in a linear, isotropic material take the form

$$\begin{aligned}\nabla\times\mathbf{H}^{tot}&=-i\omega\epsilon\mathbf{E}^{tot},\\ \nabla\times\mathbf{E}^{tot}&=i\omega\mu\mathbf{H}^{tot},\end{aligned}\tag{1}$$

where $\mathbf{E}^{tot}$ and $\mathbf{H}^{tot}$ are the total electric and magnetic fields. ϵ is the permittivity of the medium and μ its permeability. We are mainly interested in dielectric inclusions embedded in a background medium, but will consider perfect conductors briefly at the end of this section. The total fields $(\mathbf{E}^{tot},\mathbf{H}^{tot})$ can be written as the sums of the incident fields $(\mathbf{E}^{in},\mathbf{H}^{in})$, defined only in the exterior region, and scattered fields $(\mathbf{E},\mathbf{H})$ defined in both the inclusions and the exterior:

$$\begin{aligned}\mathbf{E}^{tot}&=\mathbf{E}^{in}+\mathbf{E},\\ \mathbf{H}^{tot}&=\mathbf{H}^{in}+\mathbf{H}.\end{aligned}\tag{2}$$

It is well-known [17,23] that at dielectric interfaces, the Maxwell Eqs. (1) are uniquely solvable when supplemented by the the continuity conditions:

$$\begin{aligned}\left[\mathbf{n}\times\mathbf{E}^{tot}\right]=\mathbf{0}&\Rightarrow\left[\mathbf{n}\times\mathbf{E}\right]=-\left[\mathbf{n}\times\mathbf{E}^{in}\right]\\ \left[\mathbf{n}\times\mathbf{H}^{tot}\right]=\mathbf{0}&\Rightarrow\left[\mathbf{n}\times\mathbf{H}\right]=-\left[\mathbf{n}\times\mathbf{H}^{in}\right]\end{aligned}\tag{3}$$

and the Silver–Müller radiation conditions on the scattered field. The expression $[\mathbf{n}\times\mathbf{F}]$ is used to denote the jump in the tangential components of the vector field $\mathbf{F}$ at a point on the interface.

2.1. Debye potentials

About a century ago, Debye [6], Lorenz [18] and Mie [20] independently solved the problem of scattering from a single sphere by using separation of variables. Without entering into the derivation, it is straightforward to verify that

$$\mathbf{E}(\mathbf{x}) = \nabla \times \nabla \times (\mathbf{x}v(\mathbf{x}) + i\omega\epsilon\nabla \times (\mathbf{x}u(\mathbf{x}))$$
$$\mathbf{H}(\mathbf{x}) = \nabla \times \nabla \times (\mathbf{x}u(\mathbf{x})) - i\omega\mu\nabla \times (\mathbf{x}v(\mathbf{x})) \tag{4}$$

represent an electromagnetic field, where $\mathbf{x}$ denotes the position vector with respect to the sphere center, so long as the *Debye potentials* u, v satisfy the scalar Helmholtz equation

$$\Delta u + k^2 u = 0, \quad \Delta v + k^2 v = 0,$$

with Helmholtz parameter (wave number) $k^2 = \omega^2\epsilon\mu$. In the exterior of a sphere, the Debye potentials u, v can be represented by the multipole expansions

$$u^{ext}(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} b_{n,m}h_n(kr)Y_n^m(\theta,\phi)$$
$$v^{ext}(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} a_{n,m}h_n(kr)Y_n^m(\theta,\phi) \tag{5}$$

where (r,θ,ϕ) are the spherical coordinates of the point $\mathbf{x}$ with respect to the sphere center, $h_n(r)$ is the spherical Hankel function of order n, and $Y_n^m(\theta,\phi)$ is the usual spherical harmonic of order n and degree m. The resulting electromagnetic field then also satisfies the appropriate radiation conditions at infinity. In the interior of a sphere, u and v can be represented by the local expansions

$$u^{int}(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} d_{n,m}j_n(kr)Y_n^m(\theta,\phi)$$
$$v^{int}(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} c_{n,m}j_n(kr)Y_n^m(\theta,\phi) \tag{6}$$

where $j_n(x)$ is the spherical Bessel function of order n.

Remark 2.1. To improve readability, we will abbreviate

$$\sum_{n=0}^{\infty}\sum_{m=-n}^{n} \quad \text{as} \quad \sum_{n,m}$$

and the truncated sum

$$\sum_{n=0}^{p}\sum_{m=-n}^{n} \quad \text{as} \quad \sum_{n,m}^{p}.$$

It is straightforward to verify that the total number of terms in the truncated summation is $(p+1)^2$.

2.2. Single sphere scattering

Suppose now that one is interested in scattering from a single dielectric sphere S of radius R with permittivity ϵ_1, permeability μ_1, and Helmholtz parameter $k_1 = \sqrt{\omega^2\epsilon_1\mu_1}$, in response to an incoming field $(\mathbf{E}^{in}, \mathbf{H}^{in})$. The external medium is assumed to have permittivity ϵ_0, permeability μ_0, and Helmholtz parameter $k_0 = \sqrt{\omega^2\epsilon_0\mu_0}$. Then the scattered field can be represented by (4) with $k = k_1$ in (6) for (r,θ,ϕ) inside S and by (4) with $k = k_0$ in (5) for (r,θ,ϕ) outside S.

Let us denote by $\mathbf{E}_0, \mathbf{H}_0$ the scattered field in the exterior domain and by $\mathbf{E}_1, \mathbf{H}_1$ the scattered field inside S. Then

$$\mathbf{E}_0(\mathbf{x}) = \sum_{n,m} a_{n,m}\nabla \times \nabla \times (\mathbf{x}\phi_{n,m}^{k_0}) + i\omega\mu_0\sum_{n,m} b_{n,m}\nabla \times (\mathbf{x}\phi_{n,m}^{k_0})$$
$$\mathbf{H}_0(\mathbf{x}) = \sum_{n,m} b_{n,m}\nabla \times \nabla \times (\mathbf{x}\phi_{n,m}^{k_0}) - i\omega\epsilon_0\sum_{n,m} a_{n,m}\nabla \times (\mathbf{x}\phi_{n,m}^{k_0})$$

where $\phi_{n,m}^k(\mathbf{x}) = \phi_{n,m}^k[r,\theta,\phi] = h_n(kr)Y_n^m(\theta,\phi)$ and

$$\mathbf{E}_1(\mathbf{x}) = \sum_{n,m} c_{n,m}\nabla \times \nabla \times (\mathbf{x}\psi_{n,m}^{k_1}) + i\omega\mu_1\sum_{n,m} d_{n,m}\nabla \times (\mathbf{x}\psi_{n,m}^{k_1})$$
$$\mathbf{H}_1(\mathbf{x}) = \sum_{n,m} d_{n,m}\nabla \times \nabla \times (\mathbf{x}\psi_{n,m}^{k_1}) - i\omega\epsilon_1\sum_{n,m} c_{n,m}\nabla \times (\mathbf{x}\psi_{n,m}^{k_1})$$

where $\psi_{n,m}^k(\mathbf{x}) = \psi_{n,m}^k[r,\theta,\phi] = j_n(kr)Y_n^m(\theta,\phi)$.

We may also expand $(\mathbf{E}^{in}, \mathbf{H}^{in})$ in terms of spherical harmonics on the surface of S:

$$\mathbf{E}^{in}(\mathbf{x}) = \sum_{n,m} \alpha_{n,m} \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}) + i\omega\mu_0 \sum_{n,m} \beta_{n,m} \nabla \times (\mathbf{x}\psi^{k_0}_{n,m})$$
$$\mathbf{H}^{in}(\mathbf{x}) = \sum_{n,m} \beta_{n,m} \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}) - i\omega\epsilon_0 \sum_{n,m} \alpha_{n,m} \nabla \times (\mathbf{x}\psi^{k_0}_{n,m})$$

All of the spherical harmonic modes uncouple for fixed n, m, allowing for the determination of $(a_{n,m}, b_{n,m}, c_{n,m}, d_{n,m})$ from the data $(\alpha_{n,m}, \beta_{n,m})$ by applying the interface conditions (3). After some algebra (see, for example, [3,21]), one obtains two uncoupled linear systems of the form

$$\begin{pmatrix} H_n(k_0R) & -J_n(k_1R) \\ \epsilon_0 h_n(k_0R) & -\epsilon_1 j_n(k_1R) \end{pmatrix} \begin{pmatrix} a_{n,m} \\ c_{n,m} \end{pmatrix} = \begin{pmatrix} -J_n(k_0R)\alpha_{n,m} \\ -\epsilon_0 j_n(k_0R)\alpha_{n,m} \end{pmatrix} \tag{7}$$

$$\begin{pmatrix} H_n(k_0R) & -J_n(k_1R) \\ \mu_0 h_n(k_0R) & -\mu_1 j_n(k_1R) \end{pmatrix} \begin{pmatrix} b_{n,m} \\ d_{n,m} \end{pmatrix} = \begin{pmatrix} -J_n(k_0R)\beta_{n,m} \\ -\mu_0 j_n(k_0R)\beta_{n,m} \end{pmatrix} \tag{8}$$

where $H_n(z) = [h_n(z) + zh'_n(z)]$, $J_n(z) = [j_n(z) + zj'_n(z)]$.

Definition 2.1. The mapping from incoming coefficients $(\alpha_{n,m}, \beta_{n,m})$ to the outgoing coefficients $(a_{n,m}, b_{n,m})$ is referred to as the scattering matrix and denoted by S.

2.3. Perfect conductors

If the sphere S is a perfect conductor, the corresponding boundary conditions are that the tangential components of the total electric field are zero [17,23]:

$$\mathbf{n} \times \mathbf{E}^{tot} = \mathbf{0} \Rightarrow \mathbf{n} \times \mathbf{E} = -\mathbf{n} \times \mathbf{E}^{in}. \tag{9}$$

In that case, the interior field is identically zero and the scattered matrix is given by

$$a_{n,m} = -(J_n(k_0R)/H_n(k_0R))\alpha_{n,m}$$
$$b_{n,m} = -(j_n(k_0R)/h_n(k_0R))\beta_{n,m} \tag{10}$$

3. Scattering from multiple spheres

Suppose now that one is interested in scattering from M disjoint dielectric spheres, where each sphere S_l has radius R_l and $k_l = \sqrt{\omega^2\epsilon_l\mu_l}$. The external medium and incoming field are as above. Then, the incoming field can be represented on the surface of S_l by the expansion

$$\mathbf{E}^{in}_l = \sum_{n,m} \alpha^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\psi^{k_0}_{n,m}(\mathbf{x}_l)) + i\omega\mu_0 \sum_{n,m} \beta^l_{n,m} \nabla \times (\mathbf{x}_l\psi^{k_0}_{n,m}(\mathbf{x}_l))$$
$$\mathbf{H}^{in}_l = \sum_{n,m} \beta^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\psi^{k_0}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_0 \sum_{n,m} \alpha^l_{n,m} \nabla \times (\mathbf{x}_l\psi^{k_0}_{n,m}(\mathbf{x}_l)),$$

while the scattered field in the interior of S_l can be represented by the expansion

$$\mathbf{E}_l = \sum_{n,m} c^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\psi^{k_l}_{n,m}(\mathbf{x}_l)) + i\omega\mu_l \sum_{n,m} d^l_{n,m} \nabla \times (\mathbf{x}_l\psi^{k_l}_{n,m}(\mathbf{x}_l)) \tag{11}$$

$$\mathbf{H}_l = \sum_{n,m} d^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\psi^{k_l}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_l \sum_{n,m} c^l_{n,m} \nabla \times (\mathbf{x}_l\psi^{k_l}_{n,m}(\mathbf{x}_l)). \tag{12}$$

Here, $\psi^k_{n,m}(\mathbf{x}_l) = j_n(kr_l)Y^m_n(\theta_l, \phi_l)$ is computed in terms of the spherical coordinates (r_l, θ_l, ϕ_l) of a point $\mathbf{x}_l$ with respect to the center of S_l.

The scattered field in the exterior of all the spheres can be represented by a sum of outgoing expansions, one centered on each sphere:

$$\mathbf{E}_0 = \sum_{l=1}^{M} \sum_{n,m} a^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\phi^{k_0}_{n,m}(\mathbf{x}_l)) + i\omega\mu_0 \sum_{l=1}^{M} \sum_{n,m} b^l_{n,m} \nabla \times (\mathbf{x}_l\phi^{k_0}_{n,m}(\mathbf{x}_l))$$
$$\mathbf{H}_0 = \sum_{l=1}^{M} \sum_{n,m} b^l_{n,m} \nabla \times \nabla \times (\mathbf{x}_l\phi^{k_0}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_0 \sum_{l=1}^{M} \sum_{n,m} a^l_{n,m} \nabla \times (\mathbf{x}_l\phi^{k_0}_{n,m}(\mathbf{x}_l)),$$

where $\phi^{k_0}_{n,m}(\mathbf{x}_l) = h_n(k_0 r_l) Y^m_n(\theta_l, \phi_l)$. In the preceding expression, we assume that the target, say $\mathbf{x}$, has spherical coordinates $\mathbf{x}_l = (r_l, \theta_l, \phi_l)$ with respect to the center of sphere S_l. The coefficients $(a^l_{n,m}, b^l_{n,m}, c^l_{n,m}, d^l_{n,m})$ are all unknowns. They are determined by a linear system that imposes the dielectric interface condition (3) on each sphere boundary. Unlike the case of a single sphere, however, it is no longer trivial to solve for these unknowns, since the incoming field experienced on each sphere is due, not only to the known incoming field $(\mathbf{E}^{in}, \mathbf{H}^{in})$, but to the field scattered by all the other spheres. This results in a dense linear system involving all of the unknowns, whose solution accounts for all of these *multiple scattering* interactions.

3.1. Translation operators for multiple scattering

Fortunately, the outgoing Debye expansion on sphere S_j can be analytically converted to an incoming expansion on sphere S_l for $l \neq j$.

Lemma 1. *Let the outgoing expansion from sphere S_j be given by*

$$\mathbf{E}^j_0 = \sum_{n,m} a^j_{n,m} \nabla \times \nabla \times (\mathbf{x}_j \phi^{k_0}_{n,m}(\mathbf{x}_j)) + i\omega\mu_0 \sum_{n,m} b^j_{n,m} \nabla \times (\mathbf{x}_j \phi^{k_0}_{n,m}(\mathbf{x}_j))$$
$$\mathbf{H}^j_0 = \sum_{n,m} b^j_{n,m} \nabla \times \nabla \times (\mathbf{x}_j \phi^{k_0}_{n,m}(\mathbf{x}_j)) - i\omega\epsilon_0 \sum_{n,m} a^j_{n,m} \nabla \times (\mathbf{x}_j \phi^{k_0}_{n,m}(\mathbf{x}_j)).$$

Then, the corresponding field induced on the surface of sphere S_l can be represented in the form

$$\mathbf{E}^l_0 = \sum_{n,m} \gamma^{j,l}_{n,m} \nabla \times \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) + i\omega\mu_0 \sum_{n,m} \delta^{j,l}_{n,m} \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l))$$
$$\mathbf{H}^l_0 = \sum_{n,m} \delta^{j,l}_{n,m} \nabla \times \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_0 \sum_{n,m} \gamma^{j,l}_{n,m} \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)).$$

We denote the mappings from the $\{a^j_{n,m}\}$ and $\{b^j_{n,m}\}$ coefficients to the $\{\gamma^{j,l}_{n,m}\}$ and $\{\delta^{j,l}_{n,m}\}$ coefficients by $T^{a,\gamma}_{j,l}, T^{b,\gamma}_{j,l}$, $T^{a,\delta}_{j,l}$, and $T^{b,\delta}_{j,l}$, respectively. Each of these mappings depends on the vector from the center of sphere S_j to sphere S_l and the parameters $(\mu_0, \epsilon_0, \omega)$.

For convenience, we will sometimes denote vectors of coefficients such as $\{a^j_{n,m}\}$ by $\vec{a^j}$. The individual components of a translated vector such as $T^{a,\delta}_{j,l}\vec{a^j}$ will be denoted by $[T^{a,\delta}_{j,l}\vec{a^j}]_{n,m}$.

Remark 3.1. The formulae for the *translation operators* $T^{a,\gamma}_{j,l}, T^{b,\gamma}_{j,l}, T^{a,\delta}_{j,l}$, and $T^{b,\delta}_{j,l}$ are rather involved [8,11,21]. If the expansions are truncated at $n = p$ terms, there are $2(p+1)^2$ nonzero coefficients in both the outgoing $(a^j_{n,m}, b^j_{n,m})$ and incoming $(\gamma^{j,l}_{n,m}, \delta^{j,l}_{n,m})$ representations. Each translation operator is dense and, therefore requires $O(p^4)$ operations to apply. More efficient schemes [11,1,7,9,16,25,27] reduces the cost to $O(p^3)$, while the diagonal-form of the FMM [5,24] reduces the cost to $O(p^2 \log p)$ for well-separated spheres in the high-frequency regime.

Let us now assume that all outgoing and incoming expansion are truncated at $n = p$ terms. The choice of p is determined by accuracy considerations. It must be sufficiently large to resolve the **E** and **H** fields on each sphere surface to the desired precision.

Using the preceding lemma, the total field immediately exterior to sphere S_l can be written in the form

$$\mathbf{E}^l_0 = \mathbf{E}^{in}_l + \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\gamma}_{j,l}\vec{a^j} + T^{b,\gamma}_{j,l}\vec{b^j}]_{n,m} \nabla \times \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) + i\omega\mu_0 \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\delta}_{j,l}\vec{a^j} + T^{b,\delta}_{j,l}\vec{b^j}]_{n,m} \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) + \sum_{n,m}^{p} a^l_{n,m} \nabla \times \nabla$$
$$\times (\mathbf{x}_l \phi^{k_0}_{n,m}(\mathbf{x}_l)) + i\omega\mu_0 \sum_{n,m}^{p} b^l_{n,m} \nabla \times (\mathbf{x}_l \phi^{k_0}_{n,m}(\mathbf{x}_l)) \tag{13}$$

$$\mathbf{H}^l_0 = \mathbf{H}^{in}_l + \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\delta}_{j,l}\vec{a^j} + T^{b,\delta}_{j,l}\vec{b^j}]_{n,m} \nabla \times \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_0 \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\gamma}_{j,l}\vec{a^j} + T^{b,\gamma}_{j,l}\vec{b^j}]_{n,m} \nabla \times (\mathbf{x}_l \psi^{k_0}_{n,m}(\mathbf{x}_l)) + \sum_{n,m}^{p} b^l_{n,m} \nabla \times \nabla$$
$$\times (\mathbf{x}_l \phi^{k_0}_{n,m}(\mathbf{x}_l)) - i\omega\epsilon_0 \sum_{n,m}^{p} a^l_{n,m} \nabla \times (\mathbf{x}_l \phi^{k_0}_{n,m}(\mathbf{x}_l)). \tag{14}$$

The first terms in the preceding expressions for $\mathbf{E}^l_0, \mathbf{H}^l_0$ account for the incoming field, while the next two terms account for the scattered field coming from all other spheres. The last two terms in each expression account for the fields being scattered by S_l itself.

It is now clear how to apply the interface conditions (3). We simply equate the tangential components of $\mathbf{E}^l_0, \mathbf{H}^l_0$ defined in (13), (14) with the tangential components of the interior representations $(\mathbf{E}_l, \mathbf{H}_l)$ defined in (11), (12). This yields a dense linear system of dimension $4M(p+1)^2$ for the coefficients $(a^l_{n,m}, b^l_{n,m}, c^l_{n,m}, d^l_{n,m})$. We will refer to this system as the *multiple scattering equations*. Writing the equations out explicitly is not especially informative, and we omit it.

Remark 3.2. The scattering matrix $\mathcal{S}$ (Definition 2.1) allows for the elimination of the interior variables $(c^l_{n,m}, d^l_{n,m})$, so that one can solve a modified system of dimension $2M(p+1)^2$ for the coefficients $(a^l_{n,m}, b^l_{n,m})$ describing the exterior field alone.

$$\begin{pmatrix} a^l_{n,m} \\ \\ b^l_{n,m} \end{pmatrix} = \mathcal{S} \begin{pmatrix} \alpha^l_{n,m} + \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\gamma}_{j,l} \vec{a^j} + T^{b,\gamma}_{j,l} \vec{b^j}]_{n,m} \\ \\ \beta^l_{n,m} + \sum_{\substack{j=1 \\ j\neq l}}^{M} [T^{a,\delta}_{j,l} \vec{a^j} + T^{b,\delta}_{j,l} \vec{b^j}]_{n,m} \end{pmatrix} \tag{15}$$

It is worth emphasizing that the multiple scattering equations are hardly new. There is a vast literature on the subject, which we do not seek to review here. We refer the reader to the textbooks [2,3,13,19,21] and the papers [11,27].

3.2. Iterative solution of the multiple scattering problem for a system of spheres

We will solve the multiple scattering equations iteratively, using GMRES [26] with a block diagonal preconditioner, each block corresponding to the unknowns on a single sphere. In applying the preconditioner, we simply invert each of the M diagonal blocks, which corresponds to solving the single sphere scattering problem described in Section 2.2. Since all M spheres interact, however, the system matrix is dense. Each matrix–vector multiply in the iterative solution process, if carried out naively, would require $O(M^2p^3)$ work.

In order to accelerate the solution procedure, the wideband fast multipole method (FMM) [5] can easily be modified to reduce the cost to $O(Mp^3)$ work per iteration. This is discussed in the context of acoustic scattering in [12,14]. Since the literature on FMMs is substantial, we omit a detailed discussion of the technique, but present results in Section 6.

4. Scattering from an arbitrary structure

Suppose now that instead of a sphere, we are given a smooth substructure (which may involve more than one component), denoted by D_1. For the sake of simplicity, we assume each component of D_1 has permittivity ϵ_1 and permeability μ_1 and that D_1 is embedded in the same infinite medium as above. We will suppose further that D_1 can be enclosed in a sphere S_1 (Fig. 2). As before, at the material interface, the conditions to be satisfied are (3). The Debye-Lorenz–Mie formalism cannot be applied in this case, and attempts to do so (called the T-matrix method) suffer from ill-conditioning when D_1 is sufficiently non-spherical. We, therefore, turn to the standard representation of electromagnetic fields in general geometries, based on the vector and scalar potentials and anti-potentials [22,23,28].

The vector potential in domain l ($l = 0, 1$) is defined by

$$\mathbf{A}_l(\mathbf{x}) = \epsilon_l \mu_l \int_{\partial D_1} g_l(\mathbf{x}-\mathbf{y}) \mathbf{J}(\mathbf{y}) ds_{\mathbf{y}}$$

and $g_l(\mathbf{x}) = e^{ik_l\|\mathbf{x}\|}/(4\pi\|\mathbf{x}\|)$ with $k_l = \sqrt{w^2\epsilon_j\mu_j}$. When the argument of the square root is complex, k_l is taken to lie in the upper half-plane. We define the vector anti-potential in domain l by

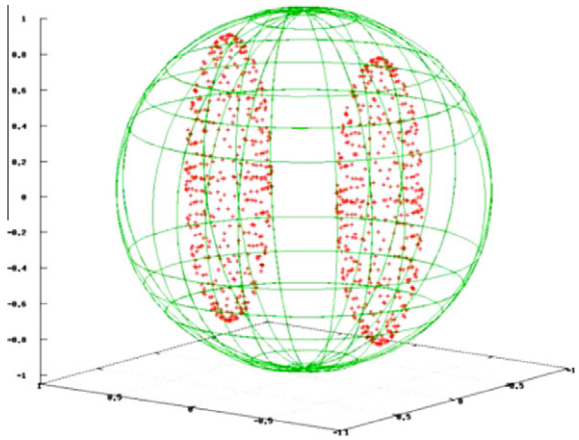

Fig. 2. A pair of triangulated ellipsoids define a bounded domain D_1 that lies with an enclosing sphere S_1. The scattering matrix for D_1 will be created on S_1 and used to represent the exterior field.

$$\tilde{\mathbf{A}}_l(\mathbf{x}) = \epsilon_l \mu_l \int_{\partial D_1} g_l(\mathbf{x}-\mathbf{y})\mathbf{K}\, ds.$$

From these, we may write

$$\mathbf{E}_l = -\nabla \phi_l + i\omega \mathbf{A}_l - \frac{1}{\epsilon_l}\nabla \times \tilde{\mathbf{A}}_l \tag{16}$$

$$\mathbf{H}_l = \frac{1}{\mu_l}\nabla \times \mathbf{A}_l - \nabla \psi_l + i\omega \tilde{\mathbf{A}}_l. \tag{17}$$

where

$$\phi_l = \frac{1}{i\omega\epsilon_l\mu_l}\nabla \cdot \mathbf{A}_l$$

$$\psi_l = \frac{1}{i\omega\epsilon_l\mu_l}\nabla \cdot \tilde{\mathbf{A}}_l.$$

We assume that **J** and **K** are surface currents, each with two tangential components. Thus, we have four degrees of freedom at each point $P \in \partial D_1$, and four boundary conditions (the continuity of the tangential components of **E** and **H**). Imposing the conditions (3) on **J**, **K** results in a resonance-free Fredholm equation of the second kind, so long as ϵ, μ and k lie in the closed upper half of the complex plane.

In more detail, using the facts that

$$\nabla_{\mathbf{x}} \times (g_l(\mathbf{x}-\mathbf{y})\mathbf{K}(\mathbf{y})) = \nabla_{\mathbf{x}} g_l \times \mathbf{K}(\mathbf{y}),$$

$$a \times b \times c = b(a \cdot c) - c(a \cdot b),$$

and, for $\mathbf{y}_0 \in \partial D_1$,

$$\lim_{\substack{\mathbf{x}\to\mathbf{y}_0 \\ \mathbf{x}\in D_0}} \int_{\partial D_1} \frac{\partial g_l}{\partial n_{\mathbf{y}_0}}(\mathbf{x}-\mathbf{y})\sigma(\mathbf{y})ds_{\mathbf{y}} = -\frac{1}{2}\sigma(\mathbf{y}_0) + \oint_{\partial D_1} \frac{\partial g_l}{\partial n_{\mathbf{y}_0}}(\mathbf{y}_0-\mathbf{y})\sigma(\mathbf{y})ds_{\mathbf{y}}$$

$$\lim_{\substack{\mathbf{x}\to\mathbf{y}_0 \\ \mathbf{x}\in D_1}} \int_{\partial D_1} \frac{\partial g_l}{\partial n_{\mathbf{y}_0}}(\mathbf{x}-\mathbf{y})\sigma(\mathbf{y})ds_{\mathbf{y}} = +\frac{1}{2}\sigma(\mathbf{y}_0) + \oint_{\partial D_1} \frac{\partial g_l}{\partial n_{\mathbf{y}_0}}(\mathbf{y}_0-\mathbf{y})\,\sigma(\mathbf{y})ds_{\mathbf{y}},$$

we obtain the following coupled set of equations.

$$\begin{aligned} -\mathbf{n}\times\mathbf{E}^{in} = {} & i\omega \int_{\partial D_1} [\epsilon_0\mu_0 g_0 - \epsilon_1\mu_1 g_1](\mathbf{n}\times\mathbf{J})\, ds_{\mathbf{y}} + \frac{i}{\omega}\mathbf{n}\times\int_{\partial D_1}[\nabla\nabla g_0 - \nabla\nabla g_1]\mathbf{J}ds_{\mathbf{y}} - \int_{\partial D_1}[\mu_0\nabla g_0 - \mu_1\nabla g_1] \\ & \times(\mathbf{n}\cdot\mathbf{K})ds_{\mathbf{y}} - \left(\frac{\mu_0+\mu_1}{2}\right)\mathbf{K} + \oint_{\partial D_1}\left(\mu_0\frac{\partial g_0}{\partial n} - \mu_1\frac{\partial g_1}{\partial n}\right)\mathbf{K}ds_{\mathbf{y}} \end{aligned} \tag{18}$$

$$\begin{aligned} -\mathbf{n}\times\mathbf{H}^{in} = {} & i\omega \int_{\partial D_1} [\mu_0\epsilon_0 g_0 - \epsilon_1\mu_1 g_1](\mathbf{n}\times\mathbf{K})\, ds_{\mathbf{y}} + \frac{i}{\omega}\mathbf{n}\times\int_{\partial D_1}[\nabla\nabla g_0 - \nabla\nabla g_1]\mathbf{K}ds_{\mathbf{y}} + \int_{\partial D_1}[\epsilon_0\nabla g_0 - \epsilon_1\nabla g_1](\mathbf{n}\cdot\mathbf{J})ds_{\mathbf{y}} \\ & + \left(\frac{\epsilon_0+\epsilon_1}{2}\right)\mathbf{J} - \oint_{\partial D_1}\left[\epsilon_0\frac{\partial g_0}{\partial n} - \epsilon_1\frac{\partial g_1}{\partial n}\right]\mathbf{J}ds_{\mathbf{y}}. \end{aligned} \tag{19}$$

The equation above is, in some sense, the dual of Müller's integral equation [22], in which the unknowns chosen are the tangential components of **E**, **H** themselves, derived from the Stratton–Chu representation. Because the Eqs. (18, 19) form a system of second kind Fredholm equations, the order of accuracy of the solution is that of the underlying quadrature rule. For first order accuracy, we assume **J** and **K** are piecewise constant current densities on a flat triangulated surface. For second order accuracy, we assume **J** and **K** are piecewise linear current densities on a piecewise quadratic surface with each curved triangle defined by six points (Fig. 3). Higher order accurate codes are obtained by increasing the order of approximation of both the surface and the current densities.

For each discretization node, we evaluate the relevant electromagnetic field component using a mixture of analytic and numerical quadratures on each triangle. More precisely, we use the method of singularity subtraction - computing integrals analytically for the kernel $1/r$ and its derivatives and using numerical quadrature for the *difference kernel* $[e^{ikr}-1]/r$, which is smoother. This results in a complex linear system of dimension $4N \times 4N$ for first order accuracy and of dimension $12N \times 12N$ for second order accuracy, where N denotes the number of triangles. For small N, say $N < 1000$, one can use direct LU-factorization to solve the linear system. For larger values of N, iterative solution with FMM-acceleration becomes much more practical [5].

Fig. 3. In the simplest geometric model, the surface of the scatterer ∂D_1 is approximated by a collection of flat triangles, defined by the locations of its three vertices in $\mathbb{R}^3$. On each triangle, there are two linearly independent tangent directions $\mathbf{t}_1$ and $\mathbf{t}_2$. The unknown electric and magnetic currents $\mathbf{J}$ and $\mathbf{K}$ on each triangle are defined by $j_1\mathbf{t}_1 + j_2\mathbf{t}_2$ and $k_1\mathbf{t}_1 + k_2\mathbf{t}_2$, respectively, and the electromagnetic fields are evaluated at the triangle centroids. For higher order accuracy, each quadratic surface patch is specified by six nodes: the three triangle vertices and three additional points, one on each curved triangle side. Three "support nodes" $\mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^3$ are then selected in the interior of each patch. Our representation for $\mathbf{J}$ and $\mathbf{K}$ at each support node $\mathbf{x}^i$ is of the form $j_1^i\mathbf{t}_1^i + j_2^i\mathbf{t}_2^i$ and $k_1^i\mathbf{t}_1^i + k_2^i\mathbf{t}_2^i$, where $\mathbf{t}_1^i, \mathbf{t}_2^i$ are linearly independent tangent vectors at $\mathbf{x}^i$. The support nodes are also the points where we evaluate the electromagnetic fields and impose interface conditions.

4.1. The scattering matrix for D_1

Suppose now that we are interested in scattering from the two ellipsoids D_1 shown in Fig. 2 due to an incoming field which is regular in the enclosing sphere S_1. Such an incoming field can be expanded within S_1 in the form

$$\mathbf{E}^{in}(\mathbf{x}) = \sum_{n,m} \alpha_{n,m} \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}) + i\omega\mu_0 \sum_{n,m} \beta_{n,m} \nabla \times (\mathbf{x}\psi^{k_0}_{n,m})$$
$$\mathbf{H}^{in}(\mathbf{x}) = \sum_{n,m} \beta_{n,m} \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}) - i\omega\epsilon_0 \sum_{n,m} \alpha_{n,m} \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}),$$

as in Section 2.2. Each (vector) spherical harmonic modes, corresponding to a single $\alpha_{n,m}$ or $\beta_{n,m}$, defines a particular incoming field on D_1. More precisely, we can solve the second kind Müller–like Eqs. (18, 19) for a right-hand side obtained by setting the incoming field to be

$$\mathbf{E}^{in}_{\alpha,n,m}(\mathbf{x}) = \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}), \quad \mathbf{H}^{in}_{\alpha,n,m}(\mathbf{x}) = -i\omega\epsilon_0 \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}), \tag{20}$$

corresponding to setting a fixed $\alpha_{n,m} = 1$ and all other coefficients to zero. Similarly, we can set the incoming field to be

$$\mathbf{E}^{in}_{\beta,n,m}(\mathbf{x}) = +i\omega\mu_0 \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}), \quad \mathbf{H}^{in}_{\beta,n,m}(\mathbf{x}) = \nabla \times \nabla \times (\mathbf{x}\psi^{k_0}_{n,m}) \tag{21}$$

corresponding to setting a fixed $\beta_{n,m} = 1$ and all other coefficients to zero. We can then store either the electric and magnetic currents $\mathbf{J}^{\alpha,n,m}, \mathbf{K}^{\alpha,n,m}, \mathbf{J}^{\beta,n,m}, \mathbf{K}^{\beta,n,m}$ induced by these (unit) incoming fields or just convert these currents to the coefficients of the outgoing (scattered) fields:

$$\mathbf{E}^{sc}_{\alpha,n,m}(\mathbf{x}) = \sum_{n',m'} a^{\alpha,n,m}_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) + i\omega\mu_0 \sum_{n',m'} b^{\alpha,n,m}_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'})$$

$$\mathbf{H}^{sc}_{\alpha,n,m}(\mathbf{x}) = \sum_{n',m'} b^{\alpha,n,m}_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) - i\omega\epsilon_0 \sum_{n',m'} a^{\alpha,n,m}_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'})$$

and

$$\mathbf{E}^{sc}_{\beta,n,m}(\mathbf{x}) = \sum_{n',m'} a^{\beta,n,m}_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) + i\omega\mu_0 \sum_{n',m'} b^{\beta,n,m}_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'})$$

$$\mathbf{H}^{sc}_{\beta,n,m}(\mathbf{x}) = \sum_{n',m'} b^{\beta,n,m}_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) - i\omega\epsilon_0 \sum_{n',m'} a^{\beta,n,m}_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}).$$

The formula for converting the currents $\mathbf{J}^{\alpha,n,m}, \mathbf{K}^{\alpha,n,m}, \mathbf{J}^{\beta,n,m}, \mathbf{K}^{\beta,n,m}$, to the coefficients can be obtained by orthogonal projection of the induced field on the enclosing sphere [23].

By superposition, an incoming field defined by the vector of incoming coefficients $\{\alpha_{n,m}, \beta_{n,m}\}$ results in a scattered field of the form

$$\mathbf{E}^{sc}(\mathbf{x}) = \sum_{n',m'} a_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) + i\omega\mu_0 \sum_{n',m'} b_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'})$$
$$\mathbf{H}^{sc}(\mathbf{x}) = \sum_{n',m'} b_{n',m'} \nabla \times \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}) - i\omega\epsilon_0 \sum_{n',m'} a_{n',m'} \nabla \times (\mathbf{x}\phi^{k_0}_{n',m'}),$$

with the coefficients of the scattered field given by

$$a_{n',m'} = \sum_{n,m} \alpha_{n,m} a^{\alpha,n,m}_{n',m'} + \beta_{n,m} a^{\beta,n,m}_{n',m'}$$
$$b_{n',m'} = \sum_{n,m} \alpha_{n,m} b^{\alpha,n,m}_{n',m'} + \beta_{n,m} b^{\beta,n,m}_{n',m'}.$$

The matrix mapping the incoming to the scattered coefficients is referred to as the *scattering matrix* for the structure D_1.

Fixing the order of the expansions above at p, there are $2p^2 + 4p$ possible basis functions that span the space of all possible incoming fields. We must, therefore solve $2p^2 + 4p$ integral equations on the detailed geometry defining D_1. To store the currents induced by each incoming field requires $O(Np^2)$ memory, where N denotes the number of degrees of freedom used in the discretization of the integral equation. The scattering matrix itself requires storing $(2p^2 + 4p)^2$ complex numbers. While somewhat expensive, these can be viewed as pre-computation steps, in anticipation of simulating materials with thousands or millions of substructures of the same identical shape, but well enough separated that the scattering matrices are accurate. The parameter p must be sufficiently large to resolve the incoming and outgoing fields on S_1. For modest separation of S_1 from D_1, the error decays exponentially as p increases.

5. Multiple scattering from well-separated non-spherical structures

Once the scattering matrix is known, the solution to the full Maxwell equations for geometries with N substructures ($N = 200$ in Fig. 1) can be turned into a multiple-scattering problem based only on the enclosing spheres. That is, the substructures can be replaced by their scattering matrices and the multiple scattering method of Section 3 can be used with trivial modifications.

There are two distinct advantages to be gained here. First, we have reduced the number of degrees of freedom from, say, 5000 or 10,000 unknown current density values per substructure to, say, 400 expansion coefficients. Just as important, however, is that we have precomputed the solution operator for each substructure in isolation, so that the linear system we solve by iteration on the multi-sphere system is much more well-conditioned. Further, the FMM reduces the cost of each iteration from $O(N^2)$ to $O(N \log N)$ and is particularly efficient here, since the complicated quadratures on triangulated surfaces have been subsumed into the precomputation step.

The principal limitations of the method are (1) that some modest separation distance between substructures is required and (2) that the bookkeeping becomes a bit awkward if more than a few distinct nanoparticle types are allowed. In many experimental settings, both conditions are satisfied.

It is worth noting that the method of this paper can be viewed as a *reduced order model* for the scattering problem. In broad terms, the idea is not new and there is substantial activity in this area in both electromagnetics and other fields (see, for example, [4]). It is also worth noting that the method is "rigorous" in the sense that the error is determined in a straightforward manner by the accuracy of the integral equation solver and the order of expansion of the scattering matrix. It fails (or needs local modification) if and only if two enclosing spheres intersect.

6. Numerical examples

As discussed in Section 4, the Müller–like integral equation is an effective method for determining the scattering matrix from a dielectric structure of arbitrary shape. To illustrate its performance, we consider the geometry in Fig. 2, consisting of a pair of ellipsoids triangulated with piecewise quadratic triangles on which we allow piecewise linear current densities. The lengths of the major and minor axes of the ellipsoids are $0.88 \times 0.29 \times 0.29$ and the separation between them is 0.47. The enclosing sphere is of unit radius and the wavelength is chosen to be 2π. We use the values $\epsilon_1 = (0.467 + 2.415i)^2$, $\mu_1 = 1$ and $\epsilon_0 = \mu_0 = 1$ for D_1 and the exterior region, respectively. Each triangle has three nodes with two degrees of freedom for each current (electric and magnetic) at each point. With 180 triangles, the resulting linear system is of dimension 2160×2160. Creating the matrix requires about 1 s. A dense matrix based iterative solver (using GMRES) then requires 0.1 s for each possible incoming mode, With $p = 3$, there are a total of 30 such modes in the scattering matrix.

With 720 and 2800 triangles, the linear systems have dimension 8640 and 34,560, respectively. Forming the dense matrix requires 11 s. in the first case and 160 s. in the latter. The iterative solution times for each incoming mode is 3.5 s in the first case and 87 s in the latter. We could accelerate these solution times using fast multipole-based codes (or any of a variety of other "fast" algorithms), but we view this cost as an initialization step and the CPU times are acceptable. The errors are of the order $10^{-3}, 10^{-4}$, and 10^{-5} for the successively finer discretizations, somewhat better than the expected second order convergence. (All calculations and timings reported in this section have been carried out using a 12-core 2.93 GHz Intel Xeon workstation, with OpenMP directives in the FMPS code.)

Remark 6.1. We have used a simple and robust test for estimating the accuracy of the integral equation method. Rather than solve the true scattering problem, we can define interior and exterior electromagnetic fields due to fictitious sources. That is, for $\mathbf{x} \in D_1$, we assume the field is due to known electric and magnetic current dipoles located in the exterior region. Likewise, for $\mathbf{x}$ in the exterior, we assume the field is due to known electric and magnetic current dipoles located within D_1. We can

then generate artificial jumps in the tangential components of $\mathbf{E}, \mathbf{H}$ and solve for $\mathbf{J}, \mathbf{K}$ to annihilate those jumps. The fields induced by $\mathbf{J}, \mathbf{K}$ can then be compared to the known analytic solution at any target. We have also used standard self-consistent error estimation. Both approaches yield errors of the magnitude listed above.

Remark 6.2. The electric and magnetic fields are computed at any point from (16, 17). This step, too, can be accelerated with the FMM, with some care taken in quadrature for target points that are close to the interface. For target points outside the enclosing sphere, of course, it is more efficient to use the scattering representation (3).

To illustrate the performance of the FMPS algorithm, we consider a $21 \times 21 \times 2$ array of scatterers, each consisting of an ellipsoid pair with a scattering matrix of order $p = 3$ derived from the integral Eqs. (18, 19). Using the same 12-core 2.93 GHz Intel Xeon workstation, the time required was about 2 s per iteration, with six iterations required for GMRES to converge to 3 digits. The "slow" multiple scattering (SMPS) approach, without fast multipole acceleration, required about 7 s per iteration. For a $21 \times 21 \times 4$ array, the cost was about 6 s per iteration (28 s for SMPS) and for a $21 \times 21 \times 8$ array, the cost was about 23 s per iteration (108 s for SMPS). For a $21 \times 21 \times 16$ array (14,112 ellipsoid pairs), the cost was about 59 s per iteration (440 s for SMPS).

The reason for the modest speedup of the FMPS over the SMPS approach is that the number of spheres is still rather small. For one million scatterers, the speedup factor would be about 1000. Careful readers may note that the FMPS scaling appears worse than $O(N \log N)$ in successively doubling the simulation from a $21 \times 21 \times 4$ array to a $21 \times 21 \times 8$ array to a $21 \times 21 \times 16$ array. For those familiar with the FMM, the short explanation is that the "near neighbor" cost is not yet in the asymptotic regime in the first two cases. Timings extrapolated from the last case are accurate for any volume-filling distribution.

7. Conclusions

The FMPS method introduced in this paper (fast multi-particle scattering) combines an integral equation solver with multiple scattering theory, in order to permit the solution to the full Maxwell equations in configurations typical of engineered composites. We assume that the geometry consists of a large number of scattering substructures embedded in a homogeneous background, assuming only that the permeabiliities, permittivities and wavenumber lie in the closed upper half of the complex plane. This avoids the possibility of (non-physical) resonances in the inclusions.

While we have only included a single type of substructure (a nanorod pair) in our examples above, it is clear that the method can easily be applied to allow for several such types, so long as there is a modest separation between substructures. FMPS is enormously faster than a full FMM-based solver using the full discretization of the geometry. With 14,112 ellipsoid pairs (the largest example in the preceding section), this would require about 30 million degrees of freedom, many minutes per iteration, and many more iterations.

In its present form, the method cannot be used for tightly packed configurations, since the multiple scattering formalism assumes that the embedding spheres are not overlapping. This can be overcome using more elaborate fast direct solvers [10,15]. FMPS does, however, permit workstation-based simulation with millions of inclusions. We are currently working on extending the method so that it can handle inclusions embedded in a layered medium.

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