A mesh-free approach to acoustic scattering from multiple spheres nested inside a large sphere by using diagonal translation operators

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A multiple-scattering approach is presented to compute the solution of the Helmholtz equation when a number of spherical scatterers are nested in the interior of an acoustically large enclosing sphere. The solution is represented in terms of partial-wave expansions, and a linear system of equations is derived to enforce continuity of pressure and normal particle velocity across all material interfaces. This approach yields high-order accuracy and avoids some of the difficulties encountered when using integral equations that apply to surfaces of arbitrary shape. Calculations are accelerated by using diagonal translation operators to compute the interactions between spheres when the operators are numerically stable. Numerical results are presented to demonstrate the accuracy and efficiency of the method. © 2010 Acoustical Society of America. [DOI: 10.1121/1.3277219]

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I. INTRODUCTION

The efficient calculation of scattering from inhomogeneities embedded in an acoustically large domain is of interest in a variety of applications. This paper is restricted to the case of spherical inclusions contained within a large sphere, because this defines a rich class of simply described model problems. That is, the geometry and material properties require only the specification of the center locations, radii, sound speeds, densities, and attenuation parameters. Such geometries serve, for example, as useful models for inverse scattering algorithms.^{1–4}

An application of particular interest is the estimation and correction of aberration through human tissue.^{5–7} Tissue-mimicking phantoms are often used to study this problem under controlled circumstances that are clinically relevant. Spheres are attractive components of laboratory phantoms because the shapes are easy to make and have been shown to mimic the aberration behavior observed in human tissue.⁶ A single enclosing medium keeps the sphere locations fixed relative to each other and mimics the properties of background tissue. A frequency-domain algorithm that computes scattering from spherical objects in the presence of an enclosing medium allows for the systematic evaluation of the performance of inverse scattering methods, with straightforward experimental validation of the forward model as well.

To be concrete, the modeling of ultrasound wave scattering by a spherical phantom 48 mm in diameter is consid-

ered. Inside this phantom are 12 smaller spheres designed to mimic the properties of human fat, skin, and muscle tissue. Laboratory measurements are conducted by immersing the phantom in water and transmitting temporal pulses with a center frequency of 2.5 MHz. At this frequency, the diameter of the outer sphere is approximately $80\lambda_0$, where λ_0 is the wavelength in water. Calculation of scattering by this large outer sphere with several smaller inclusions is a challenging problem that demands efficient methods.

An important approach to the scattering problem for general geometries in two or three dimensions is based on integral-equation formulations accelerated by the fast multipole method (FMM).^{8–12} In full, hierarchical implementations, the FMM reduces the cost of application of the integral operator from $O(N^2)$ to $O(N \log N)$ or $O(N)$, where N is the number of discrete elements used to model the scatterer surfaces.¹¹ However, robust solvers that are high-order accurate require substantial meshing efforts, quadratures for singular integrals, and care to ensure that the integral equation is numerically well-conditioned. While FMM-based solvers have been applied to general scattering problems involving tens of millions of unknowns,^{12,13} specialized techniques that take advantage of the scattering geometry to reduce the number of unknowns can improve efficiency and performance. In the case of spheres, partial-wave expansions^{14,15} obviate many of the issues that complicate general-purpose solvers.

In the computational literature, the use of partial-wave expansions is often referred to as the *T*-matrix approach,^{16–18} and is based simply on defining the linear relationship between incoming and outgoing waves, centered on each scatterer, that satisfy the physical interface conditions. These re-

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relationships are diagonal when fields are expressed in terms of spherical harmonic expansions. In an iterative solution process, one basically updates the outgoing waves by computing the incoming fields due to all of the other scattering expansions based on the current iteration. Since the “self-interaction” on each sphere is in diagonal form, the bulk of the work consists of converting the outgoing expansions emanating from each scatterer into incoming expansions centered on all of the others.

When large numbers of small scatterers are involved, FMM-based schemes are natural candidates. Previous research has produced effective schemes that borrow at least some FMM concepts, such as T -matrix approaches, multipole expansions, and efficient translation operators.^{19–21} The methods implemented in these papers employ rotation operators and recurrence relations to efficiently evaluate the required translation operators. This “rotate-shift-rotate” approach is substantially more efficient than direct translation of spherical harmonics, but is less effective in the presence of a large enclosing sphere.

This paper presents a T -matrix method for solving the scattering problem using a formulation similar to that of Ref. 19. Boundary conditions are imposed on the surface of each scatterer, and a linear system is solved to calculate the scattered field, expressed through a partial-wave expansion centered on each sphere. In the spherical harmonic basis, the modes on a single sphere are uncoupled, so that the self-interaction of each sphere is simply diagonal. Unlike general-purpose integral-equation methods, no geometric meshing or singular integrals are encountered, and high-order accuracy is straightforward to achieve. Thus, the number of degrees of freedom required on each sphere is modest, dependent only on its acoustic size and, more weakly, on its separation distance from other scatterers.

Despite the broad similarities, this work differs from Ref. 19 in three ways. First, the translation of scattered fields between spheres is accomplished using diagonal forms²² rather than the rotate-shift-rotate approach, reducing the cost of each translation from $O(p^3)$ to $O(p^2 \log p)$, where p is the degree of the partial-wave expansion.²³ Second, this paper examines the more complicated problem of scattering from small inclusions embedded in an acoustically large phantom which may be tens or hundreds of wavelengths in diameter. Third, the problem formulation uses interface conditions that match both the pressure and normal particle velocity across the inclusion boundaries. Ensuring the continuity of these physical parameters results in wave behavior that replicates the interaction of acoustic waves with soft tissue, parametrized in terms of sound speed, absorption, and density. The analysis of Refs. 19 and 20 relied on impedance boundary conditions, which provide a convenient mathematical formalism for describing the fast algorithm, but are not adequate as a physical model in the present setting.

Of these three, the introduction of an enclosing medium is the most interesting new feature, allowing the calculation of scattering due to actual tissue-mimicking phantoms realizable in the laboratory. The addition of the enclosing sphere requires augmentation of the system of equations with additional unknowns to account for the additional material inter-

face. The number of unknowns is proportional to the surface area of the enclosing sphere measured in wavelengths and is typically much larger than the number of unknowns associated with each small scatterer.

As a technical matter, the diagonal translation operators employed in this method suffer from numerical instability if the distance over which the translation is carried out is too small. Under such conditions, the rotate-shift-rotate approach of Ref. 19 is prescribed in place of diagonal translations. This happens infrequently, when spheres are within a wavelength of each other or so. A detailed analysis of the issue is presented in this paper.

Finally, note that the existence of the diagonal form lies at the heart of the FMM for high-frequency scattering, as explained in detail in Ref. 23. However, the model problems of interest did not require a full implementation of the FMM. Computational costs of this method are dominated by interaction between the enclosing phantom and the small scatterers rather than interactions between the small scatterers themselves. If the number of inclusions in the model were increased by an order of magnitude or more, then the recommended approach would be to couple a scheme like that of Ref. 20 with the analytic tools discussed here.

II. THEORY

The problem of acoustic scattering from an arbitrary medium characterized by a spatially varying complex sound speed $c(\mathbf{r})$ is considered. The imaginary part of the sound speed describes the loss in the medium. If all pressure fields have frequency ω and an $e^{-i\omega t}$ time dependence, the total pressure field $\varphi(\mathbf{r})$ satisfies the Helmholtz equation

$$[\nabla^2 + k^2(\mathbf{r})]\varphi(\mathbf{r}) = 0, \quad (1)$$

where the wavenumber $k = \omega/c$. The total pressure is

$$\varphi(\mathbf{r}) = \xi(\mathbf{r}) + \varphi_s(\mathbf{r}), \quad (2)$$

where ξ is a known incident field and φ_s is the field scattered by the medium. The scattered field satisfies the Sommerfeld radiation condition,

$$\lim_{r \rightarrow \infty} [\partial_r \varphi_s - ik\varphi_s] = 0, \quad (3)$$

where $r = |\mathbf{r}|$. The boundary conditions between two distinct homogeneous regions require continuity of total pressure and normal particle velocity across the interface Γ separating the two regions. Hence,

$$\varphi_1(\mathbf{r}) = \varphi_2(\mathbf{r}), \quad \mathbf{r} \in \Gamma, \quad (4a)$$

$$\partial_n \varphi_1(\mathbf{r}) = \rho_r \partial_n \varphi_2(\mathbf{r}), \quad \mathbf{r} \in \Gamma, \quad (4b)$$

where $\rho_r = \rho_1/\rho_2$. In the i -th medium, the pressure is $\varphi_i(\mathbf{r})$ and the density is ρ_i . The direction n of differentiation in Eq. (4b) is that of the outward normal to Γ at the point $\mathbf{r}$.

A. Scattering from a single sphere

Scattering from a single homogeneous sphere of radius a embedded in a homogeneous background material is most simply described when the center of the sphere is placed at

the origin of a spherical coordinate system with coordinate vectors of the form $\mathbf{r}=(r, \theta, \phi)$. The boundary of the sphere is described by the set of points

$$\Gamma=\{\mathbf{r}:r=a\}. \quad (5)$$

With this description, the normal n coincides with the unit radial vector $\mathbf{e}_r$. The interior of the sphere supports a regular pressure wave $\varphi_2(\mathbf{r})$, while the exterior of the sphere supports a pressure $\varphi_1(\mathbf{r})=\xi(\mathbf{r})+\varphi_s(\mathbf{r})$ consisting of a regular incident wave and an outgoing, singular scattered field.

The use of spherical harmonic expansions for all field components makes evaluation of the boundary conditions straightforward. Because the incident and internal waves are both regular, they have regular harmonic expansions. The expansion of the incident field is limited to the outside of the sphere, while the expansion of the internal wave is valid only inside the sphere. The scattered field is defined outside of the sphere by a harmonic expansion that is singular at the origin. Taking into account these constraints, the harmonic expansions of the field components are

$$\xi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^l\chi_{lm}j_l(k_1r)Y_{lm}(\theta,\phi), \quad r>a, \quad (6a)$$

$$\varphi_s(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^lB_{lm}h_l(k_1r)Y_{lm}(\theta,\phi), \quad r>a, \quad (6b)$$

$$\varphi_2(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^lC_{lm}j_l(k_2r)Y_{lm}(\theta,\phi), \quad r<a, \quad (6c)$$

where χ_{lm} , B_{lm} , and C_{lm} are coefficients of their respective harmonic expansions. The function $Y_{lm}(\theta, \phi)$ represents the spherical harmonic of degree l and order m , h_l is a spherical Hankel function of the first kind of order l , j_l is a spherical Bessel function of order l , and k_i is the wavenumber in the i -th medium. The boundary conditions (4) can be reduced to a series of well-known scattering quotients^{14,15} Q_l mapping coefficients of the incident field (6a) to those of the scattered field (6b) without concern for the internal field (6c),

$$B_{lm}=\frac{\gamma j_l(k_1a)j_l'(k_2a)-j_l'(k_1a)j_l(k_2a)}{h_l'(k_1a)j_l(k_2a)-\gamma h_l(k_1a)j_l'(k_2a)}\chi_{lm}=Q_l\chi_{lm}, \quad (7)$$

where $\gamma=\rho_1k_2/\rho_2k_1$ and the prime indicates differentiation of the Bessel functions with respect to their whole arguments. Because each scattering quotient Q_l in Eq. (7) maps an incoming spherical harmonic coefficient to exactly one outgoing coefficient of the same degree and order, the scattering operator is diagonal. Calculation of the scattering of incoming waves is, therefore, as efficient as possible.

B. Multiple spheres

When N disjoint scattering spheres are considered, scattering quotients such as those in Eq. (7) can be computed with slight modifications. The field outside of all spheres can be represented as the superposition of a known incident field ξ and scattered fields radiating from each object,

$$\varphi_0(\mathbf{r})=\xi(\mathbf{r})+\sum_{i=1}^N\varphi_{s,i}(\mathbf{r}). \quad (8)$$

Let S_i denote the i -th sphere, which has center $\mathbf{c}_i$, wavenumber k_i , density ρ_i , and radius a_i . The regular wave inside the sphere S_i will be denoted φ_i . The scattered fields $\varphi_{s,i}$ are singular at the centers of the spheres. The incident, scattered, and internal fields have the respective expansions

$$\xi(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^l\chi_{lm}^ij_l(k_0r_i)Y_{lm}(\theta_i,\phi_i), \quad r_i>a_i, \quad (9a)$$

$$\varphi_{s,i}(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^lB_{lm}^ih_l(k_0r_i)Y_{lm}(\theta_i,\phi_i), \quad r_i>a_i, \quad (9b)$$

$$\varphi_i(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^lC_{lm}^ij_l(k_ir_i)Y_{lm}(\theta_i,\phi_i), \quad r_i<a_i, \quad (9c)$$

where (r_i, θ_i, ϕ_i) represents the spherical coordinates of the vector $\mathbf{r}_i=\mathbf{r}-\mathbf{c}_i$.

The scattered fields $\varphi_{s,j}$ are regular within sphere S_i whenever $i \neq j$. Therefore, within S_i , the field $\varphi_{s,j}$ has a spherical harmonic expansion that can be expressed as

$$\varphi_{s,j}(\mathbf{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^lD_{lm}^{ij}j_l(k_ir_i)Y_{lm}(\theta_i,\phi_i), \quad r_i<a_i, \quad (10)$$

in which the regular wave coefficients D_{lm}^{ij} are translations of the singular wave coefficients B_{lm}^j from sphere S_j to S_i . The boundary conditions (4) can be used with the expansions (9) and (10) to relate the scattered-field coefficients B_{lm}^i to the translated coefficients D_{lm}^{ij} and the coefficients χ_{lm}^i of the incident field. Because spherical harmonics are orthogonal, the boundary conditions split into equations of the form

$$I_{lm}^ij_l(ka_i)+B_{lm}^ih_l(ka_i)=C_{lm}^ij_l(k_ia_i), \quad (11a)$$

$$I_{lm}^ij_l'(ka_i)+B_{lm}^ih_l'(ka_i)=\gamma C_{lm}^ij_l'(k_ia_i), \quad (11b)$$

where k is the wavenumber of the background medium and $\gamma_i=\rho_0k_i/\rho_ik$. The regular wave coefficients

$$I_{lm}^i=\chi_{lm}^i+\sum_{j \neq i}D_{lm}^{ij} \quad (12)$$

describe the total wave impinging on sphere S_i . This wave is the superposition of the incident field and the scattered fields from all spheres S_j distinct from S_i . The solution of the system (11) provides scattering quotients for the sphere S_i ,

$$B_{lm}^i=\frac{\gamma j_l(ka_i)j_l'(k_ia_i)-j_l'(ka_i)j_l(k_ia_i)}{h_l'(ka_i)j_l(k_ia_i)-\gamma h_l(ka_i)j_l'(k_ia_i)}I_{lm}^i=Q_l^ij_{lm}^i. \quad (13)$$

The coefficients Q_l^i in Eq. (13) are equivalent to those in Eq. (7), except that the incident field coefficients χ_{lm}^i are replaced by the regular wave coefficients I_{lm}^i representing all fields incident upon S_i . In an iterative approach based on the T -matrix method, each iteration of the solution uses coefficients I_{lm}^i derived from the fields computed in the previous iteration to produce new scattered-field coefficients B_{lm}^i .

C. Translations of spherical harmonics

The keystone of the spherical scattering operator with coefficients defined in Eq. (13) is a translator that converts and recenters singular harmonic expansions of the form (9b) to regular wave expansions of the form (10). The translator is developed from the addition theorem for spherical harmonics.^{24,25} This theorem relates a singular spherical harmonic to a linear combination of regular harmonics,

$$h_l(kr)Y_{lm}(\theta, \phi) = \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \alpha_{l'm'lm}(k, \mathbf{r}'') j_{l'}(kr') Y_{l'm'}(\theta', \phi'), \quad (14)$$

where $\mathbf{r} = \mathbf{r}' + \mathbf{r}''$. The translator coefficients $\alpha_{l'm'lm}$ are defined by the expression^{24,25}

$$\alpha_{l'm'lm}(k, \mathbf{r}'') = 4\pi \sum_{l''=0}^{\infty} i^{l'+l''-l} \sum_{m''=-l''}^{l''} h_{l''}(kr'') Y_{l''m''}(\theta'', \phi'') \times \int_{S_0} d\hat{s} Y_{lm}(\hat{s}) Y_{l'm'}^*(\hat{s}) Y_{l''m''}^*(\hat{s}), \quad (15)$$

where S_0 is the unit sphere. However, direct evaluation of the integral in Eq. (15) results in an inefficient, dense operation.

An efficient diagonal form of the translator (15) is the basis for the high-frequency FMM.^{22,25,26} This diagonal form may be derived from the addition theorem for the three-dimensional, free-space Green's function²⁷ expressing the field at $\mathbf{c}_j$ due to a point source located at $\mathbf{d}$ relative to the coordinate system centered on $\mathbf{c}_i$,

$$\frac{e^{ik|\mathbf{r}_{ji}+\mathbf{d}|}}{|\mathbf{r}_{ji}+\mathbf{d}|} = ik \sum_{l=0}^{\infty} (-1)^l (2l+1) j_l(kd) h_l(kr_{ji}) P_l(\hat{\mathbf{d}} \cdot \hat{\mathbf{r}}_{ji}), \quad (16)$$

where $\mathbf{r}_{ji} = \mathbf{c}_j - \mathbf{c}_i$ and P_l is the Legendre polynomial of degree l . A general vector $\mathbf{x}$ has magnitude $x = |\mathbf{x}|$ and direction $\hat{\mathbf{x}} = \mathbf{x}/x$. Taking the Fourier transform of Eq. (16) with respect to $\mathbf{d}$ yields

$$\frac{e^{ik|\mathbf{r}_{ji}+\mathbf{d}|}}{|\mathbf{r}_{ji}+\mathbf{d}|} \approx \frac{ik}{4\pi} \int_{S_0} d\hat{s} e^{ik\hat{s} \cdot \mathbf{d}} \alpha_{ji}(\hat{s}), \quad (17)$$

in which

$$\alpha_{ji}(\hat{s}) = \sum_{l=0}^L i^l (2l+1) P_l(\hat{\mathbf{r}}_{ji} \cdot \hat{\mathbf{s}}) h_l(kr_{ji}) \quad (18)$$

are the coefficients of the diagonal translation operator.

The addition theorem (16) converges as $l \rightarrow \infty$ despite the tendency for $h_l(kr_{ji})$ to approach infinity because the Bessel functions $j_l(kd)$ vanish more rapidly. However, through the Fourier transform operation and the interchange of the integration and summation, this balancing effect is lost in the diagonal form (18). Therefore, the translator sum must be truncated to a maximum number of terms, L , large enough to cause the addition theorem (16) to converge within a desired tolerance, but not large enough to cause numerical inaccuracy in Eq. (18) due to a discrepancy between the magnitudes of h_0 and h_L that exceeds the dynamic range of the chosen finite-precision arithmetic. When the translation dis-

tance r_{ji} is large compared to the radii of the source and target spheres, the excess bandwidth formula prescribes a truncation point

$$L \approx ka + 1.8d_0^{2/3}(ka)^{1/3}, \quad (19)$$

in which d_0 represents the desired number of digits of accuracy and a is the maximum of the source and target sphere radii.¹¹ Expression (19) has been found to give accurate results for electromagnetic Helmholtz problems.²⁸ The parameter L can also be computed numerically with essentially no cost²³ by analyzing the convergence of the addition theorem (16). This is necessary when the translation distance is not large compared to the radius a and the excess bandwidth formula (19) gives incorrect results.

The diagonal form of the translation operator (18) can be applied to general far-field signatures of wave fields that express the fields as coefficients of outgoing plane waves. A field $\varphi(\mathbf{r})$ has a far-field signature centered about an arbitrary point $\mathbf{a}$ that is defined by the relationship^{11,26}

$$\hat{\varphi}_a(\hat{s}) = \lim_{r \rightarrow \infty} k\tau e^{-ik\tau} \varphi(\mathbf{a} + \tau \hat{s}). \quad (20)$$

Using the large-argument approximations for Hankel functions, the scattered field $\varphi_{s,i}$ expanded according to Eq. (9b) has a far-field signature given by²³

$$\hat{\varphi}_{s,i}(\hat{s}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l (-i)^{l+1} B_{lm}^i Y_{lm}(\hat{s}). \quad (21)$$

The outgoing far-field signature (21) represents the radiation pattern, centered on $\mathbf{a} = \mathbf{c}_i$, of the sphere S_i induced by the incident field.

The translation operator (18) converts an outgoing far-field signature $\hat{\varphi}_{s,i}(\hat{s})$ for a source sphere S_i into an incident plane-wave expansion that represents the field $\varphi_{s,i}$ everywhere within a target sphere S_j . The spheres S_i and S_j must be disjoint for the translation to be valid. The coefficients $\hat{\varphi}_{ji}(\hat{s})$ of the incident plane-wave expansion are valid inside sphere S_j and are related to the outgoing far-field signature of sphere S_i by the expression

$$\hat{\varphi}_{ji}(\hat{s}) = \alpha_{ji}(\hat{s}) \hat{\varphi}_{s,i}(\hat{s}). \quad (22)$$

The incoming plane-wave expansion is related to the translated spherical harmonic expansion coefficients D_{lm}^{ji} in Eq. (10) by the expression²³

$$\hat{\varphi}_{ji}(\hat{s}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l (-i)^{l+1} D_{lm}^{ji} Y_{lm}(\hat{s}). \quad (23)$$

Hence, given the coefficients B_{lm}^i that describe a scattered field radiating outward from S_i , the translated regular wave coefficients D_{lm}^{ji} in expansion (10) can be found by converting the scattered field $\varphi_{s,i}$ to a far-field signature $\hat{\varphi}_{s,i}$, pointwise multiplying by the translator α_{ji} , and recovering the spherical harmonic expansion coefficients of the resulting incoming plane-wave expansion.

D. Spherical enclosing medium

The addition of an enclosing sphere in the description of scattering is straightforward when using partial-wave expansions. For interactions *between* interior spheres, no change to the system of equations is necessary. However, in the scattering quotients (13), the coefficients χ_{lm}^i of the known incident field must be replaced by the coefficients A_{lm} of a general spherical harmonic expansion

$$\varphi_e(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{lm} j_l(kr) Y_{lm}(\theta, \phi), \quad r < a, \quad (24)$$

that is valid within the sphere S , which has radius a , density ρ , wavenumber k , and a center $\mathbf{c}$ that coincides with the origin of the coordinate system. The coefficients A_{lm}^i represent a re-expansion of the field φ_e about the center of the sphere S_i . The recentered field is given by

$$\varphi_e(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_{lm}^i j_l(kr_i) Y_{lm}(\theta_i, \phi_i), \quad r_i < a_i, \quad (25)$$

where the coordinate variables follow the notation in Eq. (9). Since expansion (24) is valid everywhere inside the enclosing sphere S , and the internal sphere S_i is contained entirely within S , expansion (25) is valid everywhere inside S_i .

The addition of an enclosing sphere introduces two additional fields: the previously described internal field φ_e and an external scattered field $\varphi_{e,s}$. Accompanying these additional fields are two additional boundary conditions that govern the behavior of the fields at the boundary of the enclosing sphere. Those boundary conditions have the same form as boundary conditions (4) for the inner spheres. However, in this case, the external and internal fields are given by

$$\varphi_1(\mathbf{r}) = \xi(\mathbf{r}) + \varphi_{e,s}(\mathbf{r}), \quad (26a)$$

$$\varphi_2(\mathbf{r}) = \varphi_e(\mathbf{r}) + \sum_{i=1}^N \varphi_{s,i}(\mathbf{r}). \quad (26b)$$

The scattered fields $\varphi_{s,i}$ radiate outward from the spheres S_i contained within S . Hence, each field can be represented as a spherical harmonic expansion

$$\varphi_{s,i}(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l B_{lm}^{e,i} h_l(kr) Y_{lm}(\theta, \phi), \quad (27)$$

where the expansion is relative to the center of the enclosing sphere S . Since S contains S_i , expansion (27) is valid everywhere outside of S .

If the incident field has spherical harmonic expansion coefficients χ_{lm} and the external scattered field $\varphi_{e,s}$ has expansion coefficients B_{lm} , relation (26) can be employed in boundary conditions (4) with expansions (24) and (27) to provide two expressions:

$$A_{lm} = T_l \chi_{lm} + R_l \sum_{i=1}^N B_{lm}^{e,i}, \quad (28a)$$

$$B_{lm} = T_l^e \sum_{i=1}^N B_{lm}^{e,i} + R_l^e A_{lm}. \quad (28b)$$

The relation in Eq. (28a) describes the internal field φ_e as a transmission of the incident field superimposed with a reflection of the scattered fields produced by all internal spheres. Likewise, the expansion of the external field $\varphi_{e,s}$ is defined in Eq. (28b) to be the superposition of the transmission of the scattered fields produced by the internal spheres and the reflected internal field φ_e . The transmission and reflection operators appearing in Eq. (28) are given by

$$T_l = \frac{j_l'(k_0 a) h_l(k_0 a) + j_l(k_0 a) h_l'(k_0 a)}{\gamma j_l'(ka) h_l(k_0 a) - j_l(ka) h_l'(k_0 a)}, \quad (29a)$$

$$R_l = \frac{\gamma h_l(k_0 a) h_l'(ka) - h_l(ka) h_l'(k_0 a)}{\gamma j_l'(ka) h_l(k_0 a) - j_l(ka) h_l'(k_0 a)}, \quad (29b)$$

$$T_l^e = \frac{\gamma j_l(k_0 a) h_l'(ka) - j_l'(k_0 a) h_l(ka)}{j_l(k_0 a) h_l'(k_0 a) - j_l'(k_0 a) h_l(k_0 a)}, \quad (29c)$$

$$R_l^e = \frac{\gamma j_l'(ka) j_l(k_0 a) - j_l(ka) j_l'(k_0 a)}{j_l(k_0 a) h_l'(k_0 a) - j_l'(k_0 a) h_l(k_0 a)}, \quad (29d)$$

where $\gamma = \rho_0 k / \rho k_0$, with k_0 and ρ_0 , respectively, equal to the wavenumber and density of the background medium.

The field $\varphi_{e,s}$ influences neither the incident field ξ nor the internal field φ_e . The scattered fields $\varphi_{s,i}$, in turn, are influenced only by each other and the internal field φ_e . Therefore, the solution of the scattering problem can proceed without regard to the external scattered field $\varphi_{e,s}$. Once the fields φ_e and $\varphi_{s,i}$ have been computed, the external scattered field $\varphi_{e,s}$ can be computed in a single pass if desired. This reduces the computational demand of the method.

The solution of Eq. (13) requires knowledge of the shifted coefficients A_{lm}^i given the known coefficients A_{lm} . Likewise, the solution of Eq. (28a) requires shifted coefficients $B_{lm}^{e,i}$ given the known coefficients B_{lm}^i . The diagonal translation operators provide an efficient mechanism for determining these shifted coefficients.²⁶ Given the incident plane-wave expansion $\hat{\varphi}_e$ centered at the origin, the shifted incident expansion $\hat{\varphi}_e'$ centered about the point $\mathbf{c}_i$ is given by

$$\hat{\varphi}_e'(\hat{\mathbf{s}}) = e^{ik\hat{\mathbf{s}} \cdot \mathbf{c}_i} \hat{\varphi}_e(\hat{\mathbf{s}}). \quad (30)$$

This expansion is valid everywhere inside of S_i , which is wholly contained within the enclosing sphere S . Similarly, the outgoing far-field pattern $\hat{\varphi}_{s,i}'$ centered at $\mathbf{c}_i$ is related to an outgoing pattern $\hat{\varphi}_{s,i}'$ centered at the origin by

$$\hat{\varphi}_{s,i}'(\hat{\mathbf{s}}) = e^{-ik\hat{\mathbf{s}} \cdot \mathbf{c}_i} \hat{\varphi}_{s,i}(\hat{\mathbf{s}}). \quad (31)$$

The shifted far-field signature is valid outside of the enclosing sphere. The spherical harmonic expansion coefficients corresponding to the shifted incoming plane-wave expansion (30) and the outgoing far-field pattern (31) are the coefficients A_{lm}^i and $B_{lm}^{e,i}$, respectively.

The spherical harmonic expansions of each field component involve infinitely many terms. However, for practical computation, the expansions must be truncated. The trunca-

tion point is determined according to an excess bandwidth formula (19). This ensures that the fields radiating from or incident upon each field are sampled with sufficient density to accurately represent all relevant harmonic content.

For simplicity, the expansions for all internal spheres can be truncated to the same degree. However, the large outer sphere typically requires expansions of much higher degrees for accurate representation of the fields. Since the internal scattered fields $\varphi_{s,i}$ have lower degrees, their far-field patterns $\hat{\varphi}_{s,i}$ can be sampled more coarsely than the far-field patterns $\hat{\varphi}_e$ and $\hat{\xi}$. Consequently, when the patterns $\hat{\varphi}_{s,i}$ are translated to the center of the enclosing sphere, they must be more finely sampled before solving Eq. (28a). In addition, when the internal field φ_e is translated to each internal sphere for use in Eq. (13), the far-field pattern $\hat{\varphi}_e$ must be decimated after translation to match the coarser sampling grid used to define $\hat{\varphi}_{s,i}$. The methods used for decimation and interpolation are detailed in Refs. 11 and 23.

E. Iterative solution

In the absence of an enclosing sphere, equations of the form (13) for each sphere S_i , $i=1, \dots, N$, form a system of equations that describe the relationships between all field quantities. However, these relationships relate unknown coefficients B_{lm}^i to the known incident field coefficients χ_{lm}^i and the unknown coefficients D_{lm}^{ij} derived from unknown coefficients B_{lm}^j . To produce a system of equations suitable for iterative inversions, Eq. (13) must be rearranged to form

$$B_{lm}^i - Q_l^i \sum_{j \neq i} D_{lm}^{ij} = Q_l^i \chi_{lm}^i. \quad (32)$$

The resulting modified equations define a scattering map that relates the unknown coefficients B_{lm}^i for each sphere to the known coefficients of the incident field at each sphere. The scattering map is composed of both the scattering quotients Q_{lm}^i and the diagonal operators that convert outgoing coefficients B_{lm}^j into incoming coefficients D_{lm}^{ij} . The system of equations that describe the scattering map are invertible using iterative methods such as GMRES.²⁹ Convergence of the iterative scheme is monitored by tracking the residual norm associated with the solution and the scattering map.

When an enclosing sphere surrounds all inner scatterers, the equations governing the fields at the boundary of each inner scatterer are reordered to form

$$B_{lm}^i - Q_l^i \left[A_{lm}^i - \sum_{j \neq i} D_{lm}^{ij} \right] = 0. \quad (33)$$

This relationship is again derived from Eq. (13) with the previously noted exception that the coefficients χ_{lm}^i of the incident field are replaced with the coefficients A_{lm}^i of the regular field inside the enclosing sphere. The coefficients A_{lm}^i centered on S_i are related to the unknown regular field coefficients A_{lm} centered on the enclosing sphere through the diagonal translation operators (30). These unknown coefficients are related to the known incident field coefficients χ_{lm} by rearranging Eq. (28a) to yield

$$A_{lm} - R_l \sum_{i=1}^N B_{lm}^{ei} = T_l \chi_{lm}, \quad (34)$$

where the coefficients B_{lm}^{ei} centered on the enclosing sphere are related to the coefficients B_{lm}^i centered on S_i by Eq. (31). The entire system of equations consisting of Eqs. (33) and (34) form a scattering map that relates all unknown quantities to the known incident field coefficients using the three diagonal translation operators and the scattering quotients Q_{lm} . This map may be inverted using GMRES in a manner similar to that for the case involving no enclosing sphere.

F. Comparison to the fast multipole method

The fundamental aspects of the fast multipole method are efficient diagonal forms for translation operators and aggregation and distribution procedures. The aggregation procedure collects far-field signatures of individual scattering elements into a source group signature that is translated using diagonal forms to a target group of scattering elements. The translated signature is then distributed to individual elements within the target group. Modern, hierarchical implementations further reduce computational demand.^{11,23} The name “fast multipole method” for high-frequency scattering reflects the use of diagonal translation operators, which are Fourier transforms of translation operators for multipole (spherical harmonic) expansions.

The method presented to compute scattering from spheres uses the same diagonal translation operators employed in the FMM. However, because the number of spheres considered in the numerical studies was not large, aggregation and distribution of fields for groups of scattering elements were unnecessary. Consequently, application of the name “fast multipole method” to the presented approach is not appropriate. Instead, the described method is called the “sphere multipole method” to emphasize the use of spheres as scattering elements and the use of spherical harmonic (multipole) expansions to represent fields.

III. NUMERICAL RESULTS

Three examples are presented to illustrate the accuracy and efficiency of the method. The first example consists of simple problems involving two spheres at various distances that demonstrate the accuracy of translation even for short distances. The second example is a larger problem involving 12 spheres with differing material properties that exhibits increased efficiency over an algorithm using dense translations. In the third example, the 12 spheres are embedded in an enclosing sphere to form a geometry resembling a tissue-mimicking phantom that is used for aberration estimation.

A. Two spheres

Two tests each considered scattering from two spheres immersed in water. The sound speed in the water was 1509 m/s and the density was 997 kg/m³. The sound speed in each sphere was 1613 m/s with an attenuation slope of 1.61 dB/cm MHz and a density equal to that of water. The two spheres were separated along the y axis and the incident

FIG. 1. (Color online) Azimuthal and polar scattering patterns for two spheres, each with a 2 mm radius, separated by 10 mm center to center. The excitation frequency was 2.5 MHz.

plane wave was traveling in the $-y$ direction at a frequency of 2.5 MHz. The results were compared to simulations using a volume integral-equation method that requires a meshed representation of the scattering geometry.

In the first calculation, two spheres with 2 mm radii were separated by 10 mm. The scattering patterns of the two spheres are shown in Fig. 1 along with the results from the reference simulation. The large separation between the spheres ensures that the scattering pattern is accurately computed. The mean-squared error (MSE) between the fields computed by the fast multiple-scattering method and the integral-equation method is defined as

$$\text{MSE} = \left[\int_{\Omega} d\hat{s} |\varphi_s(\hat{s}) - \varphi_{s,r}(\hat{s})|^2 \right] / \left[\int_{\Omega} d\hat{s} |\varphi_{s,r}(\hat{s})|^2 \right]^{1/2}, \quad (35)$$

where Ω is the unit sphere, φ_s is the scattered field computed with the fast multiple-scattering method, and $\varphi_{s,r}$ is the reference scattered field computed with the integral-equation method. The MSE for fields shown in Fig. 1 is 2.4%. This error reflects inaccuracies due to truncation of the field components and diagonal translation operators in the fast method in addition to discretization and numerical integration inaccuracies in the integral-equation method. If the fast method is used to compute a solution neglecting interactions between spheres (by forcing the translators to vanish in all directions), the MSE increases to 66.6%. This large increase suggests that the interactions between spheres are significant to the overall solution. The low error of the complete solution therefore provides evidence that the translators are accurate.

Two spheres with different radii and a shorter translation distance were also considered. One sphere had a radius of 2 mm, while the radius of the other sphere was 1 mm. These two spheres were separated by 3.2 mm along the y axis. Strictly speaking, this is a violation of the constraints on the use of the diagonal form that is inaccurate for scatterers in proximity. The excess bandwidth formula (19) does not correctly predict the truncation point L required for accurate evaluation of the diagonal translator, and proper selection of L according to the convergence of the addition theorem (16) results in an unstable translator. The scattered field computed

FIG. 2. (Color online) Azimuthal and polar scattering patterns for two spheres, with respective radii 1 and 2 mm, separated by 3.2 mm center to center. The excitation frequency was 2.5 MHz.

when the diagonal translator is truncated according to the excess bandwidth formula is shown in Fig. 2 to reasonably agree with the integral-equation solution. The MSE of the solution is 5.0%. When interactions between spheres are disregarded, the MSE increases to 38.1%. While this example is not as strongly influenced by interactions between spheres as the previous example, these interactions are still a significant part of the overall solution.

B. Twelve spheres

A more challenging test was posed by the geometry shown in Fig. 3. Twelve spheres, each composed of one of three materials that mimic the properties of human tissues, were embedded in a larger, contrasting sphere. The tissues and their properties are listed in Table I. The entire phantom was immersed in a background with the acoustic properties of water. The characteristics of each of the inner spheres are listed in Table II.

FIG. 3. An arrangement of 12 tissue-mimicking spheres. A spherical enclosing boundary is shown, although some tests did not consider the enclosing sphere.

TABLE I. Material properties of spheres designed to mimic human tissue.

Tissue	Sound speed (m/s)	Density (kg/m ³)	Absorption (dB/cm MHz)
Water	1509.0	997.0	0.00
Fat	1478.0	950.0	0.52
Muscle	1547.0	1050.0	0.91
Skin	1613.0	1120.0	1.61

Considering the 12 inner spheres in Fig. 3 without an enclosing sphere significantly reduces the complexity of the scattering problem. However, even without an enclosing sphere, the direct method used to validate the sphere multipole method was incapable of solving a full-scale problem with the desired excitation frequency using the available desktop computing resources. The validation method uses a matrix solver based on spherical harmonic expansions and non-diagonal harmonic translators. To produce validation results, the dimensions of the phantom were scaled uniformly by a factor of 1/3. Hence, for a sphere S_i with radius a_i and center location $\mathbf{c}_i$, the scaled sphere S'_i had radius $a'_i = a_i/3$ and center location $\mathbf{c}'_i = \mathbf{c}_i/3$. The scattering patterns shown in Fig. 4 were produced by the scaled spheres due to an incident plane wave oscillating at 2.5 MHz and traveling in the $+x$ direction. The solution was obtained in 9 s on a four-processor, shared-memory computer system using less than 200 Mbytes of memory. The MSE of the solution shown in Fig. 4 is 3.5%.

C. An enclosing sphere

Addition of the enclosing sphere surrounding the smaller tissue-mimicking spheres shown in Fig. 3 results in an accurate model of a laboratory phantom. Scattering from this structure at a range of frequencies in the neighborhood of 2.5 MHz is of interest. Simulated results are useful for equipment calibration and validation of laboratory measurements. Furthermore, the numerical results are useful for aberration correction algorithms.

When the enclosing sphere is acoustically large, the interior field must be described by a spherical harmonic expansion

TABLE II. Characteristics of the spheres in the tissue-mimicking phantom.

Radius (mm)	Center (mm)			Tissue
	x	y	z	
4.0	0.0	0.0	0.0	Fat
5.0	14.0	2.0	4.0	Skin
5.0	5.0	-10.0	-4.0	Fat
3.0	17.0	-7.0	0.0	Fat
7.8	-10.0	10.0	7.2	Muscle
7.8	5.0	12.0	-7.2	Muscle
5.0	14.0	12.0	3.0	Muscle
5.0	-5.0	-18.0	-3.0	Skin
2.5	7.5	-18.0	-2.0	Skin
1.5	-4.0	20.0	0.0	Skin
2.5	-18.0	4.0	2.0	Skin
9.1	-12.5	-5.0	-5.2	Muscle

FIG. 4. (Color online) Azimuthal and polar scattering patterns of the 12-sphere acoustic phantom (with dimensions scaled by 1/3). The excitation frequency was 2.5 MHz.

sion with a high degree. This increases the computational load of both the sphere multipole and validation methods. While the sphere multipole method is fully capable of solving the scattering problem for incident waves with frequencies in excess of 2.5 MHz, the validation code was incapable of simulating such frequencies with available resources. Thus, for validation purposes, the geometry was again reduced by a uniform scaling factor.

The 12 spheres shown in Fig. 3 were enclosed in a contrasting sphere with a radius of 24 mm. The material of the enclosing sphere had a sound speed of 1570 m/s, an attenuation slope of 0.3 dB/cm MHz, and a density of 970 kg/m³. The dimensions of the phantom were reduced by a factor of 3 to facilitate computation of validation results. An incident plane wave traveling along the $+x$ direction and a frequency of 2.5 MHz were used to excite the scaled geometry. The scattering patterns produced by the tissue-mimicking phantom in the presence of this incident wave are shown in Fig. 5 with a MSE of 6.5%. Running on four processing cores, the sphere multipole method computed a solution in 35 s using 200 Mbytes of system memory.

The sphere multipole method has also been used to simulate the enclosed, 12-sphere geometry at full scale with a much higher incident frequency. With an incident fre-

FIG. 5. (Color online) Azimuthal and polar scatter patterns for a 12-sphere acoustic phantom embedded in a contrasting enclosing sphere (with dimensions scaled by 1/3). The excitation frequency was 2.5 MHz.

FIG. 6. (Color online) Scaling of the computation times of the sphere multipole method and a direct validation technique as a function of the scaling of the geometry depicted in Fig. 3.

quency of 7.5 MHz, the sphere multipole method was able to compute a solution in 15 min with a memory consumption less than 1 Gbyte. No validation result was available for a problem of this size. These results indicate that the described method will be useful in simulating propagation through the phantom at a range of frequencies that matches those used in laboratory equipment.

D. Scaling studies

The programming environments and strategies of the implementation of the sphere multipole method and the validation codes are different. Direct comparisons between the run times of the two methods are, therefore, not meaningful. Instead, a scaling study was employed to establish the efficiency of the sphere multipole method. To perform such a study, the dimensions of the 12-sphere phantom pictured in Fig. 3 and described in Table II were reduced to various scales. The enclosing sphere was omitted because of the limitations of the validation code. Altering the geometric scale of the problem is similar to scaling the excitation frequency by the reciprocal of the geometry scaling factor. Thus, these results also describe how the algorithm scales with increasing incident frequency. However, because loss in the spheres is specified as an attenuation slope, scaling the excitation frequency alters the attenuation observed in the spheres. While this will not alter the periteration or setup times of the algorithm, different attenuation values can affect the number of iterations required for convergence.

The results of the scaling study are shown in Fig. 6. In the sphere multipole method, setup-related overhead does not depend on the number of iterations required to produce a solution. This overhead is primarily dominated by calculation of the translation operators. The iteration time reported is normalized by the minimum number of iterations required to produce a solution with a backward error less than 10^{-6} . The number of iterations increased slightly as the scale of the problem was increased. The “ideal” line shown in the figure scales as $O(L^3)$, where L is the maximum degree used in spherical harmonic expansions. The number of spheres was fixed in these studies and does not, therefore, affect the asymptotic behavior of the method.

The scaling of the direct validation method is also shown in Fig. 6. The excessively large demands on memory and computer time prevented calculation of validation results at geometric scales greater than 0.5. The validation times

FIG. 7. (Color online) The number of terms required for desired accuracy below 10^{-6} in the addition theorem for a translation $\mathbf{r}_{ji} = 1.1a\hat{x}$ and a source location $\mathbf{d} = a\hat{x}$.

have been normalized to ensure that the time observed at the minimum scale (1/32) agrees with the ideal prediction of the fast method. The figure shows that the asymptotic behaviors of the fast method and the direct method diverge rapidly. The validation method solves the same system of boundary equations solved by the sphere multipole method. However, the direct method uses dense spherical harmonic translation matrices to translate $O(L^2)$ singular wave coefficients to $O(L^2)$ regular wave coefficients. Because these matrices contain $O(L^4)$ elements, the direct method can scale no more efficiently than $O(L^4)$.

E. Truncation of the translation operator

Analyses of truncation error in the addition theorem (16) consider general distributions of point sources throughout a spherical source region of radius d . As discussed below, such considerations are not generally applicable to an analysis of translation error for fields scattered by homogeneous spheres because the harmonic bandwidth of the scattered fields is lower than that of the singular fields produced by point sources. Nevertheless, analysis of truncation error in the addition theorem illuminates worst-case concerns associated with the application of diagonal translation operators over short distances.

The addition theorem (16) is always guaranteed to converge when $d < r_{ji}$ because the Bessel term $j_l(kd)$ vanishes faster than $h_l(kr_{ji})$ increases in magnitude as l increases. However, convergence is slowest when $d = a$ and $\mathbf{d}$ is parallel or antiparallel to $\mathbf{r}_{ji}$, resulting in a Bessel term $j_l(kd)$ that vanishes slowly and a Legendre polynomial $P_l(\hat{\mathbf{d}} \cdot \hat{\mathbf{r}}_{ji})$ with maximum absolute value. The excess bandwidth formula provides a suitable estimate for the truncation point L when the translation distance r_{ji} is large relative to the source radius a . When this condition is not satisfied, a brute-force approach can be employed to directly evaluate the minimum truncation point L that ensures agreement between both sides of the addition theorem within a desired tolerance. A comparison of the truncation points computed using the excess bandwidth formula and brute-force evaluation for a translation $\mathbf{r}_{ji} = 1.1a\hat{x}$ and point-source location $\mathbf{d} = a\hat{x}$ is shown in Fig. 7 for a desired tolerance of 10^{-6} .

For short translation distances, the improved estimate of L obtained from brute-force analysis may be required to compute accurately the diagonal translation operator (18). However, when r_{ji} is small, the translator may be unstable

FIG. 8. (Color online) Estimate of the dynamic range required to accurately compute the diagonal translation operator for a translation $\mathbf{r}_{ji} = 1.1a\hat{x}$ and a source location $\mathbf{d} = a\hat{x}$.

with finite-precision arithmetic. This is because the magnitudes of the Hankel functions $h_l(kr_{ji})$ increase rapidly and monotonically when $l > kr_{ji}$. In such cases, the magnitude $|h_L(kr_{ji})|$ of the high-order term may eclipse the magnitude $|h_0(kr_{ji})|$ of the low-order term in finite-precision arithmetic. An estimate of the required dynamic range for the aforementioned translation is shown in Fig. 8 as the ratio $|h_0(kr_{ji})/h_L(kr_{ji})|$ for a desired error below 10^{-6} . When the ratio is smaller than the minimum representable number in finite-precision arithmetic, the translator sum (18) is not computed accurately.

IV. DISCUSSION

Three aspects of the described method merit special comment. The first is the truncation of and error in the diagonal translation operator. Although this topic has been discussed in considerable detail (for example, in Ref. 11), the context here is different. The number of terms required in the expansion is determined by the accuracy of the representation (9) and not by point source considerations in the standard FMM. The second issue is the computational efficiency of this method. The asymptotic complexity of the sphere multipole method depends primarily on the number of scattering spheres and their acoustic sizes. The third aspect of the sphere multipole method is the suitability of the algorithm to parallel computing.

A. Truncation of the diagonal translation operator

The worst-case estimates provided in Sec. III E assume that the scattered field radiating from a source sphere behaves as a point source located on the sphere surface. This contributes terms of high degree to the harmonic expansion of the field, but the excess bandwidth formula (19) assumes that the source and target spheres are well-separated to ensure that the source singularity is far from the target. Because high-degree harmonics are not significant in the far field, the excess bandwidth formula underestimates the harmonic content of singular source fields and prescribes a lower truncation point for the diagonal translator than necessary for near-field translations. Therefore, premature truncation of the translator according to the excess bandwidth formula results in inaccurate computation of the contributions due to high-degree components.

However, scattering from homogeneous spheres of finite radius are approximately band-limited since the scattering coefficients (13) tend to vanish rapidly as $l \rightarrow \infty$. Furthermore, the maximum harmonic degrees of all scattered fields are known as a consequence of harmonic expansions being used with diagonal scattering operators at the surface of each sphere. As discussed in Ref. 23, the harmonic bandwidth of a field is the sole determinant of the number of terms required in a diagonal translator for that field. Stability of the diagonal form is likewise dependent on the required number of terms and the translation distance, and is easily discerned from the ratio of the magnitudes of the lowest-order and highest-order terms. Even when worst-case error analysis (based on singular field assumptions) suggests that diagonal forms will be unstable for a particular source size and translation distance, the harmonic bandwidth of the source field may be sufficiently low to allow stable diagonal translation with a reduced number of terms. This phenomenon is shown in Fig. 2, where the excess bandwidth formula was used to determine the translator truncation points for short distances and the results are still accurately computed.

Because the harmonic bandwidths of all scattered fields are known during computation, and because the stability of diagonal forms is easily assessed based on the required numbers of terms and the translation distances, the cost to implement runtime checks to determine whether a given field may be accurately translated using a precomputed diagonal form is insignificant. If a check indicates that the diagonal form is not suitable for a particular translation, a rotate-shift-rotate approach^{30–32} is recommended as an alternative. This technique allows on-demand, efficient computation without the stability concerns accompanying diagonal forms. While the rotate-shift-rotate approach is less efficient than diagonal translation, the method is only required for near-neighbor translations and should not dominate the overall computational cost of the method. In the examples presented earlier, instability of the diagonal forms was not an issue, and the rotate-shift-rotate approach was not required.

B. Computational efficiency

The computational cost of the described method is heavily dependent on the maximum number of terms used in spherical harmonic expansions of fields. For simplicity, the expansion degree for each of the scattering spheres is assumed to be L , obtained either numerically or from Eq. (19). For a spherical harmonic expansion of degree L , the total number of terms in the expansion is $O(L^2)$. When the spherical harmonic expansions are transformed to far-field radiation patterns, the patterns must be sampled at $O(L^2)$ points on the unit sphere.

If scattering from N spheres is to be determined, the scattered field from each sphere must be translated to every other sphere. The total number of translations required is thus $O(N^2)$ and each translator sum (18) must be computed for $O(L^2)$ points on the unit sphere. Evaluation of the translator at a single point can be completed in $O(L)$ time. Hence,

in the simplest implementation, the overall cost for constructing the $O(N^2)$ translators is $O(N^2L^3)$. Storage of these translators requires $O(N^2L^2)$ memory.

Once the translators are constructed, their application requires only the pointwise multiplication of the far-field pattern of a field with the translator. These multiplications can be performed in $O(L^2)$ time. For a single iteration in the calculation of scattering, each translation is performed once. Hence, for each iteration, the total cost of translating far-field signatures between spheres is $O(N^2L^2)$. In contrast, each dense translation requires $O(L^4)$ time, for a total cost of $O(N^2L^4)$, while translations using a rotate-shift-rotate approach require $O(L^3)$ work for a total cost of $O(N^2L^3)$.

Application of the diagonal translation operator to interactions between scattering spheres also requires transformations between spherical harmonics and far-field signatures. With $O(L^2)$ coefficients, the far-field signature must be sampled at $O(L^2)$ distinct points on the unit sphere. Therefore, a direct evaluation of the signature (21) requires $O(L^4)$ time. However, using separation of variables,²³ the far-field signature can be evaluated in $O(L^3)$ time. A divide-and-conquer scheme has also been implemented³³ to further reduce the complexity to $O([L \log L]^2)$. A similar acceleration technique can convert an incoming plane-wave expansion (23) into a spherical harmonic expansion in $O([L \log L]^2)$ time. These transformations must be performed twice for each sphere: once to convert the field scattered from the sphere from a spherical harmonic expansion to a far-field signature and once again to convert the incoming plane-wave expansion from other spheres (which are superimposed) into a spherical harmonic expansion for scattering. Hence, the transformations can be evaluated with a complexity of $O(N[L \log L]^2)$ per iteration.

Because spherical scattering operators are diagonal, the scattering from each sphere is performed in $O(L^2)$ computer time for $O(L^2)$ spherical harmonic coefficients. A scattering operator must be applied to incoming fields centered on sphere so a total of N scattering operations must be performed. The overall cost for applying scattering operators defined in Eq. (13) is $O(NL^2)$ per iteration. This is not significant compared to the complexity of the translation operators and the spherical harmonic transformations. Hence, the overall complexity of a single iteration of the sphere multipole method can be reduced to $O(N^2L^2) + O(N[L \log L]^2)$.

If the number N of spheres is increased while the size of each sphere is kept constant, the algorithm as presented scales as $O(N^2)$. Likewise, if N is kept constant while the size of each sphere is increased (for example, by increasing the incident frequency), the algorithm scales as $O([L \log L]^2)$. The N^2 scaling issue can be overcome by a full implementation of the (hierarchical) FMM,^{10,11,20,23} reducing the cost to $O(N \log N)$ without the need to adopt an integral-equation formulation. The $[L \log L]^2$ scaling is more problematic and, for sufficiently large spheres, optimal schemes would require full integral equation approaches with FMM acceleration applied to high-order surface meshes. Nevertheless, for the medium-sized problems that are addressed in this study, the scheme of coupling “spectrally accurate” representations in a spherical harmonic basis

with efficient translation operators that generate sphere-to-sphere interactions is sufficient. For scattering spheres with very large radii (in excess of several hundred wavelengths), the additional overhead associated with a full FMM implementation is insignificant compared to the cost of the transformation between spherical harmonic expansions and far-field signatures.

The memory requirements of the fast algorithm are dominated by storage of the diagonal translators and all field coefficients. There are $O(NL^2)$ field coefficients associated with fields scattered by N spheres. The diagonal translators require storage of $O(N^2L^2)$ values for $O(N^2)$ translators. Hence, the overall storage complexity of the algorithm scales as $O(N^2L^2)$.

C. Parallel computing

The sphere multipole method can easily be made parallel with little or no synchronization overhead by using multiple threads on shared-memory systems. Both the scattering quotients in Eq. (13) and the efficient transformations between spherical harmonic expansions and outgoing far-field signatures²³ can be applied to fields radiating from each scattering sphere independently with no synchronization. In addition, translations of multipole fields between spheres can be computed in parallel, but some synchronization is required when the translated fields are used to augment the incoming wave expansion for each sphere (12) to prevent conflicting memory access between multiple threads. Distributed-memory implementations of the FMM have been developed,^{13,34,35} but care must be taken to prevent the communication demands from overshadowing the advantages of additional processors. When computing scattering at multiple frequencies for pulse excitations, a more straightforward parallel approach evaluates the solution at each desired frequency on a distinct processor. Virtually no communication or synchronization is required in such an approach.

V. CONCLUSION

A method that couples analytic expressions for scattering from a sphere with diagonal translation operators has been presented to solve the acoustic scattering problem for multiple spheres that can be enclosed within a larger sphere. Like the method of Ref. 19, a multiple-scattering formalism is used that avoids the need for discrete representation of scatterers and the evaluation of singular integrals as is typical in general-purpose integral-equation methods (with or without fast multipole acceleration). The use of diagonal translation here reduces the computational complexity involved in mapping the outgoing wave from each source sphere to each target sphere in a spherical harmonic basis. Numerical results establish the accuracy and efficiency of the new method.

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