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Mie scattering with 3D angular spectrum method

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Abstract: Mie theory is a powerful method to model electromagnetic scattering from a multilayered sphere. Usually, the incident beam is expanded to its vector spherical harmonic representation defined by beam shape coefficients, and the multilayer sphere scattering is obtained by the T-matrix method. However, obtaining the beam shape coefficients for arbitrarily shaped incident beams has limitations on source locations and requires different methods when the incident beam is defined inside or outside the computational domain or at the scatterer surface. We propose a 3D angular spectrum method for defining beam shape coefficients from arbitrary source field distributions. This method enables the placement of the sources freely within the computational domain without singularities, allowing flexibility in beam design. We demonstrate incident field synthesis and spherical scattering by comparing morphology-dependent resonances to known values, achieving excellent matching and high accuracy. The proposed method has significant benefits for optical systems and inverse beam design. It allows for the analysis of electromagnetic forward/backward propagation between optical elements and spherical targets using a single method. It is also valuable for optical force beam design and analysis.

1. Introduction

Electromagnetic scattering from a homogeneous sphere illuminated by an arbitrary incident beam can be computed with conventional methods, including full-wave simulations [1], geometrical optics [2], or physical optics [3,4]. These techniques are well-studied and accurate, given the model fidelity and a suitable wavelength range. However, they cannot assess the internal and scattered electric fields from multilayered spherical objects without considerable computational effort. Especially when the sphere’s radius is of the order of wavelengths, complete classical electromagnetic wave theory is needed [5].

Mie theory and the generalized Lorentz-Mie theory are accurate methods to evaluate the internal and scattered fields from the multilayered spheres [6–8], where the incident beam is presented in vector spherical harmonics (VSH) expansion defined by beam shape coefficients (BSCs) [9]. However, obtaining the BSCs for arbitrarily shaped incident beams can be difficult; often needing a combination of several complex methods [6,10]. BSCs can be computed from a known function or field distribution with certain constraints, such as polarization, source shape, and location limitations [11,12]. In these cases, BSCs for the incident beam are obtained by the Bromwich method [13] or multipole expansion [14–16]. These methods define the sources inside a closed volume, and the VSH expanded fields can be computed only outside of this area, limiting the source location.
BSCs can also be computed from known electric and magnetic field distributions on the surface of the spherical scatterer using closed surface orthogonality (CSO). CSO also has limitations as the fields must be defined across the entire spherical surface [17]. For example, CSO cannot be applied to fields defined only on the spherical subregion, thus excluding it from many inverse beam synthesis tasks, where the beam only illuminates a small area of the sphere [18,19]. On the other hand, BSCs can be computed from the standard 2D ASM, which does not have these location restrictions due to its eigenfunction property [20,21]. However, 2D ASM is limited to the planar surface distributions [22–24]; see the comparison of the methods in Table 1.

In this article, we adapt the curved boundary integral method (CBIM) presented in [27] to a source-free method allowing beams to propagate through the boundary surface. We simply generalize the 2D ASM for curved surfaces following the idea presented in the proof of Theorem 2.1 [27] and call this method as 3D angular spectrum method (3D ASM). The geometrical framework is the same as in [27].

We aim to create a VSH-expanded electromagnetic beam from a known electric field distribution on an arbitrarily shaped and positioned surface. Then the incident beam can be modified in terms of propagating field distribution, polarization, and local phase variation [19]. Also, the source location can be positioned inside the simulation area without restrictions. This goal can be achieved by using 3D ASM approach to accommodate arbitrary fields defined on arbitrarily shaped surfaces and construct modified BSCs for an incident beam VSH presentation.

3D ASM present the incident field in the angular spectrum domain as the sum of differently oriented plane waves. When this angular summation of plane waves on a source plane is presented in a direction cosine coordinate system, these angles can be used directly to compute the BSCs for the VSH expansion. Additionally, the internal and scattered fields from a multilayered dielectric sphere can be mapped with the extended boundary condition method (EBCM), which is referred as the T-matrix method in this article [21]. The advantages of the presented method are non-singularity at the source points, allowing the synthesis of a continuous beam through the source surface from any known electric field distribution. Finally, the incident beam can be expanded into a VSH presentation to compute scattered fields from multilayered spheres.

2. Theory

This chapter presents a method to compute the forward/backscatter of multilayered spheres under arbitrary beam illumination. The chapter is divided into three sections introducing the 3D ASM, global coordinate mapping system, and modified BSCs coefficients for the VSH expansion.

Section 2.1 derives the 3D ASM from the curved boundary integral method, which is polarized along local xz-plane and is suitable for obtaining BSCs.
Section 2.2 presents a system to map local coordinates into a global origin-centered coordinate system with each source point’s orientation and position information, which is later used to construct the BSCs.

Section 2.3 presents the VSH expansion from an arbitrary surface with modified BSCs. These BSCs are modified to include the mapped source’s orientation and position information while preserving the needed spherical symmetry for the VSH expansion.

2.1. 3D angular spectrum method

Let the global Cartesian base-vectors be \((e_x, e_y, e_z)\) in space \(\mathbb{R}^3\), where position vector is \(r = x e_x + y e_y + z e_z\) and global coordinates are marked as \(r_{\text{glob}} = (x, y, z)\). Consider a regular, compact surface \(\Omega\) in \(\mathbb{R}^3\), which has a continuously differentiable parametrization with parameters \(p\) and \(q\) as

\[
\Omega = \left\{(o(p, q) e_x + o_1(p, q) e_y + o_2(p, q) e_z) \middle| p \in [p_1, p_2], q \in [q_1, q_2]\right\}.
\]

(1)

Keeping point \(o\) as a local origin, unit vectors \(e_1, e_2\) and \(e_3\) define an orthogonal base for the local coordinate system, where \(e_1\) and \(e_2\) are in the tangent plane, and \(e_3\) is along the surface normal, see Fig. 1. Polarization is along \((e_1, e_3)\)-plane.

![Fig. 1. Vector relations between source point base-vectors on a surface and a global origin.](image)

Let vector \(r\) be presented in this base as \(r = \bar{x} e_1 + \bar{y} e_2 + \bar{z} e_3\). Its coordinate triple is marked briefly as \(r_{\text{loc}} = (\bar{x}, \bar{y}, \bar{z})\). When the vector \(r\) is expressed with both \((e_x, e_y, e_z)\) and \((e_1, e_2, e_3)\) bases, as it is known, the dependence of the coordinates on each other is determined by an orthogonal transformation matrix

\[
\Theta(p, q) = \begin{bmatrix} e_{1,\text{glob}} & e_{2,\text{glob}} & e_{3,\text{glob}} \end{bmatrix}, \quad \Theta^{-1} = \Theta^T,
\]

(2)

where the columns are the coordinate triples \(e_{1,\text{glob}}, e_{2,\text{glob}}\) and \(e_{3,\text{glob}}\). Let the position \(P\) be presented in global coordinate system as \(r = x e_x + y e_y + z e_z\). Position \(P\) presented in the local coordinate system with the global base is

\[
r - o = (x - o_x)e_x + (y - o_y)e_y + (z - o_z)e_z.
\]

(3)

Let us introduce compact notation \(\bar{r} = r - o\). The dependence of the corresponding coordinates can be written using the transformation matrix Eq. (2) as

\[
(r - o)_{\text{glob}} = \Theta \bar{r}_{\text{loc}}.
\]

(4)
Let \( E_0 \) be a continuous electric field on the surface \( \Omega \). In the article [27], we have presented integral formulas for an incident electric field created by \( E_0 \). Because our aim in this article is to utilize the Mie theory, we only use frequencies in a disc \( B(\mathbf{o};k) = \{(k_z, k_{\bar{y}}) \mid k_z^2 + k_{\bar{y}}^2 \leq k^2\} \), where \( k \) is the wavenumber. Thus, we ignore some fast-decaying ones. Accordingly, our incident electric field takes a form

\[
E(\mathbf{r}) = \frac{1}{4\pi^2} \iint_{\Omega} E_0(\mathbf{o}) [E_1(\mathbf{r}; \mathbf{o}) \mathbf{e}_1(\mathbf{o}) + E_3(\mathbf{r}; \mathbf{o}) \mathbf{e}_3(\mathbf{o})] \, d\Omega \\
= \frac{1}{4\pi^2} \iint_{\Omega} E_0(\mathbf{o}) E(\mathbf{r}; \mathbf{o}) \, d\Omega,
\]

where \( d\Omega = ||o_{\mathbf{\Omega}} \times o_{\mathbf{\Omega}}|| \, dpdq \). Moreover, the coefficient functions are

\[
E_1(\mathbf{r}; \mathbf{o}) = \int_{B(\mathbf{o};k)} e^{ik_z x + ik_{\bar{y}} y + ik_{\bar{z}} z} \, dk_z dk_{\bar{y}} dk_{\bar{z}}
\]

and

\[
E_3(\mathbf{r}; \mathbf{o}) = -\int_{B(\mathbf{o};k)} ik_z e^{ik_z x + ik_{\bar{y}} y + ik_{\bar{z}} z} \, dk_z dk_{\bar{y}} dk_{\bar{z}},
\]

where according to Eqs. ((3)–(4)) local coordinates are \((\bar{x}, \bar{y}, \bar{z}) = \bar{r}_{\text{loc}} = \Theta^T(\mathbf{r} - \mathbf{o})_{\text{glob}}, k_z = [k^2 - k_x^2 - k_{\bar{y}}^2]^{1/2}\) with the positive root and \( \mathbf{k} = k_z \mathbf{e}_1 + k_{\bar{y}} \mathbf{e}_2 + k_{\bar{z}} \mathbf{e}_3 \) is the wave vector. Furthermore, \( k = |\mathbf{k}| \). The notation \((\mathbf{r}, \mathbf{o})\) points out to electric field, related to observation point \(\mathbf{r}\), at the location point \(\mathbf{o} \in \Omega\).

Moreover, let’s denote \( s = \frac{1}{k} ||\). Hence the exponent in Eqs. (6)–(7) can be written as \( ik(k_z \bar{x} + k_{\bar{y}} \bar{y} + k_{\bar{z}} z) = \mathbf{k} \cdot \mathbf{r} = ik(\mathbf{s} \cdot \mathbf{r}) \). As in [27], the radiated electric field \( E(\mathbf{r}; \mathbf{o}) = E_1(\mathbf{r}; \mathbf{o}) \mathbf{e}_1 + E_3(\mathbf{r}; \mathbf{o}) \mathbf{e}_3 \) can be written as

\[
E(\mathbf{r}; \mathbf{o}) = \int_{B(\mathbf{o};k)} e^{ik(\mathbf{s} \cdot \mathbf{r})} \mathbf{e}_0(k_z, k_{\bar{y}}, k_{\bar{z}}) \, dk_z dk_{\bar{y}} dk_{\bar{z}},
\]

where

\[
\mathbf{e}_0(k_z, k_{\bar{y}}, k_{\bar{z}}) = \mathbf{e}_1 - \frac{k_z}{k_{\bar{y}}} \mathbf{e}_3
\]

defines polarization. The electric field presented in Eqs. (5)–(7) reduces to the standard 2D ASM representation when the surface \( \Omega \) is planar.

### 2.2. Global coordinate mapping

Equations (6)–(9) presents a electric field in the base \((\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)\). When expanding to VSH presentation, this source must be presented using position vector \(\mathbf{r}\) to preserve the spherical symmetry of VSH. Thus, a global mapping of local coordinates is needed.

We obtain according to Eq.(4) that \((\bar{x}, \bar{y}, \bar{z}) = \bar{r}_{\text{loc}} = \Theta^T(\mathbf{r} - \mathbf{o})_{\text{glob}}, k_z = [k^2 - k_x^2 - k_{\bar{y}}^2]^{1/2}\). Let’s write briefly \(\mathbf{t} = s_{\text{loc}}\) a coordinate triple of vector \(\mathbf{s}\). Consequently, we can write

\[
\mathbf{s} \cdot \bar{r} = \mathbf{t} \cdot \bar{r}_{\text{loc}} = \mathbf{t} \cdot \Theta^T(\mathbf{r} - \mathbf{o})_{\text{glob}} = \mathbf{t} \cdot (\Theta^T \mathbf{r}_{\text{glob}} - \Theta^T \mathbf{o}_{\text{glob}}) = \\
\mathbf{t} \cdot (\mathbf{r}_{\text{loc}} - \mathbf{o}_{\text{loc}}) = \mathbf{t} \cdot \mathbf{r}_{\text{loc}} - \mathbf{t} \cdot \mathbf{o}_{\text{loc}},
\]

where dot products for triples are also ordinary. Based on Eq. (10), the term \( e^{ik(\mathbf{s} \cdot \mathbf{r})} \), which is in the local coordinate system, can be presented in the global coordinate system as

\[
e^{ik(\mathbf{s} \cdot \mathbf{r})} = e^{ik(\mathbf{t} \cdot \mathbf{r}_{\text{loc}})} e^{-ik(\mathbf{t} \cdot \mathbf{o}_{\text{loc}})},
\]

where \( e^{-ik(\mathbf{t} \cdot \mathbf{o}_{\text{loc}})} = e^{-ik(\mathbf{s} \cdot \mathbf{r})} \) presents the position and phase shift of the source fields focus (waist) from global origin to the source surface. Each local field created from the source point is presented in a global coordinate system.
2.3. VSH expansion with modified beam shape coefficients

Modified BSCs coefficients for each source point are derived for presenting any parameterized field distribution in a global coordinate system, including the locations and propagation direction of the sources. These coefficients map complicated coordinate geometries into one presentation. This allows synthesizing a total electromagnetic beam as a superposition of VSH expanded fields.

Integrated wavenumbers \( k_1 \) and \( k_2 \) in Eq. (8) have direction cosine presentation analogous to the BSC angles [21]. Thus Eq. (8) is expressed in the direction cosines \( \xi \) and \( \zeta \), where \( (k \cos \xi = k_1 \) and \( k \cos \zeta = k_2 \) as

\[
E(r; o) = k^2 \int_0^{\pi} \sin \xi \left\{ \int_0^{\pi} e_0(\xi, \zeta)e^{ikt(r_{loc})}e^{-ik(t_{loc})} \sin \zeta d\zeta \right\} d\xi, \tag{12}
\]

The polarization \( e_0 \) is given as

\[
e_0(\xi, \zeta) = e_1 - \frac{\cos \xi}{(1-\cos^2 \xi - \cos^2 \zeta)^{1/2}} e_3, \tag{13}
\]

and the vector \( s \) is

\[
s = \cos \xi e_1 + \cos \zeta e_2 + (1 - \cos^2 \xi - \cos^2 \zeta)^{1/2} e_3, \tag{14}
\]

and the triple \( t \) is

\[
t = (\cos \xi, \cos \zeta, (1 - \cos^2 \xi - \cos^2 \zeta)^{1/2}) \tag{15}
\]

Then, Eq. (12) is evaluated by numerical integration using the trapezoidal rule method, which is sufficiently accurate for periodic function Eq. (12) [28], with uniform-width \( l \) [21]

\[
E(r; o) \approx (kp)^2 \sum_i \sin \xi_i \sum_j \sin \zeta \xi e_0(\xi_i, \zeta_j)e^{ik(t_{loc})}e^{-ik(t_{loc})}, \tag{16}
\]

where Eq. (11) is used. Indices \( i \) and \( j \) refer to individual plane waves with propagation constants \( k_i \) and \( k_j \), and \( p = \xi_{i+1} - \xi_i = \zeta_{j+1} - \zeta_j \) is the step size of the numerical integration.

The incident electric field can be written at an arbitrary point \( r \) by VSH expansion where local plane wave angles \((i, j)\) are converted to even and odd VSH modes \((m, n)\) as [21]

\[
E(r; o)_{inc} = (kp)^2 \sum_m \sum_n D_{mn} \left( a_{emn}^r M_{emn}^1(r) + a_{omn}^r M_{omn}^1(r) \right)
+ b_{emn}^l N_{emn}^1(r) + b_{omn}^l N_{omn}^1(r), \tag{17}
\]

where \( M_{emn}^1, M_{omn}^1, N_{emn}^1 \) and \( N_{omn}^1 \) are VSH of the first kind and \( D_{mn} \) is a normalization factor [21]. For \( kr \) we substitute spherical coordinates \((kr, \theta, \phi)\) and corresponding spherical base vectors \((e_r, e_\theta, e_\phi)\), taken with respect to the local base \((e_1, e_2, e_3)\). They can be computed from the triple \( r_{loc} \). The modified BSCs \( d_{emn}^r, d_{omn}^r, b_{emn}^l \) and \( b_{omn}^l \) are written as

\[
d_{emn}^r = \sum_j \sin \xi_j \sum_j \sin \zeta \xi d_{emn}^r e^{-ik(t_{loc})},
\]
\[
d_{omn}^r = \sum_j \sin \xi_j \sum_j \sin \zeta \xi d_{omn}^r e^{-ik(t_{loc})},
\]
\[
b_{emn}^l = \sum_j \sin \xi_j \sum_j \sin \zeta \xi b_{emn}^l e^{-ik(t_{loc})},
\]
\[
b_{omn}^l = \sum_j \sin \xi_j \sum_j \sin \zeta \xi b_{omn}^l e^{-ik(t_{loc})}.
\]

The BSCs for each \( ij \)–plane wave \( d_{emn}^r, d_{omn}^r, b_{emn}^l \) and \( b_{omn}^l \) are defined in the Appendix. Now, the incident magnetic field is obtained by rearranging the modified BSCs and by multiplying
by constant \(-i/\eta\) as

\[
\mathbf{H}(\mathbf{r}; \mathbf{o})_{\text{inc}} = -\frac{i(kp)^2}{\eta} \sum_m \sum_n D_{mn} \left[ b_{emn} M_{emn}^1(\mathbf{k} \cdot \mathbf{r}) + b_{omn} M_{omn}^1(\mathbf{k} \cdot \mathbf{r}) \right] + a_{emn} N_{emn}^1(\mathbf{k} \cdot \mathbf{r}) + a_{omn} N_{omn}^1(\mathbf{k} \cdot \mathbf{r})
\]

(19)

The total incident electric and magnetic field, accounting for polarization as in Eq. (13), is written as the integration of vector spherical harmonics expansions Eqs. (17) and (19) as

\[
\mathbf{E}(\mathbf{r})_{\text{inc}} = \frac{1}{4\pi} \iint_{\Omega} E_0(\mathbf{o}) \mathbf{E}(\mathbf{r}; \mathbf{o})_{\text{inc}} d\Omega,
\]

\[
\mathbf{H}(\mathbf{r})_{\text{inc}} = \frac{1}{4\pi} \iint_{\Omega} E_0(\mathbf{o}) \mathbf{H}(\mathbf{r}; \mathbf{o})_{\text{inc}} d\Omega.
\]

(20)

Similar scattered field presentations mapped with the T-matrix method are presented in the Appendix.

In summary, we have expanded 3D ASM incident field synthesis to the VSH expansion for obtaining Mie scattering from spherical objects. We have mapped source points’ global location and orientation information into the modified BSCs and obtained the total fields as a superposition of VSH-expanded source points. This approach satisfies the Helmholtz equation and allows us to adjust the incident field’s polarization and wavefront from the parametrization.

3. Results

The results are divided into two sections; first, we demonstrate the practicality and accuracy of the presented theory by comparing the Gaussian beam’s morphology-dependent resonances from a sphere with the traditional 2D ASM and the presented 3D ASM, and show a high degree of agreement. In the second section, we synthesize an electromagnetic beam from an ellipsoidal surface, verify the incident field with physical optics simulations, and compute scattered fields from a 100-dielectric layer sphere.

3.1. Morphology-dependent resonance test

Mie scattering region is known for frequency-dependent backscatter intensity. This phenomenon is due to the scattering resonances, which trap energy temporarily inside the sphere. Backscatter intensity is typically reported as a function of size parameter \(k\alpha\), where \(k = k_0\eta\) is the refractive index dependent wavenumber inside the sphere and \(\alpha\) is the sphere radius. These backscatter resonances are called morphology-dependent resonances (MDRs) [29,30]. MDRs are highly responsive to simulation errors and serve as a good test of the accuracy of the derived 3D ASM combined with VSH expansion [31].

To test the 3D ASM simulation accuracy, an ensemble of source points representing the Gaussian beam in [21] was defined via the 2D ASM of [32], and differences in predicted MDRs were assessed. First, a TEM\(_{00}\) beam waist was defined such that the waist was coplanar with \(z = 0\) plane and the beam centroid intersected a homogenous sphere center of curvature (plane 1 in Fig. 2) located at \((x, y, z) = (0, 0, 0)\). Then, the beam was backpropagated 5\(\alpha\) to plane 2 (Fig. 2) via the 2D ASM utilized in [32]. The field at plane 2 was discretized into a square grid of 500 \(\times\) 500 points. Source points generated via the 3D ASM were placed at these points, and the field magnitude, phase, polarization, and Poynting vector were defined by the 2D ASM computed field. The fields were then propagated from plane 2 to the sphere via 3D ASM, and backscatter intensity was analyzed at a point on the optical axis \((x, y, z) = (0, 0, -500\alpha)\) as the size parameter range was tuned from 32 to 36. Backscatter at this point was also computed via 2D ASM from plane 1. Finally, the backscatter from a single source point on the axis at plane 2 \((0, 0, -5\alpha)\) was
Fig. 2. Morphology-dependent resonance simulation of a sphere illuminated by Gaussian beam. On a) is a Gaussian beam synthesis on the source Plane 1 at the origin, and field components are computed on Plane 2. On b) is Simulation 2, where Plane 2 is used as a 3D ASM source, where each source point’s local propagation direction is defined by the local Poynting vector (marked as blue), and source points are multiplied by complex amplitudes, obtained from Simulation 1.

Fig. 3. Simulation flow graph.

also assessed at \((0, 0, -500\alpha)\) to demonstrate the difference between a single source point and the source point ensemble.

The coated sphere simulations were done in the same way, except that the beam axis was placed tangential to the outer coating surface. The waist (plane 1) was still coplanar with the \(z = 0\) plane, but the beam centroid was displaced vertically to \(y = \alpha\). This configuration couples to whispering gallery-like modes, and discrepancies in the predicted MDRs are even more sensitive to simulation error than the above-described homogeneous sphere configuration. See simulation flow with source planes 1 and 2 in Fig. 3.

Simulations are executed by illuminating homogeneous and coated spheres by Gaussian beam in size parameter range \(k\alpha \in [32, 36]\) with beam waist radius \(\omega_0 = 1.5\lambda\). Homogeneous spheres have a refractive index of \(n_r = 1.36\), and coated spheres have a \(n_r = 1.36\) core with a \(n_c = 1.5\) shell with radius of \(0.7\alpha\). These values were selected from article [32] for comparing results.
Fig. 4. Electric and magnetic field components of Gaussian beam one at the plane 2. On a)-c) are electric field components, and on d)-f) are magnetic field components. All the components are normalized by \( \max |E_x| \).

The Cartesian electric and magnetic field components of the incident field at plane 2 are presented in Fig. 4. These components are synthesized from plane 1.

Gaussian beam MDRs synthesized from both source plane scenarios are computed at -500 \( \alpha \) distance from the origin [21] and compared in Fig. 5.

Fig. 5. Morphology-dependent resonances of a Gaussian beam. On a) is a Gaussian beam focused at the origin of the homogeneous sphere with refractive index \( n_r = 1.36 \). On b) is a Gaussian beam focused on the side \( y = \alpha \) of the coated sphere, with a core refractive index of \( n_r = 1.5 \) and shell as \( n_r = 1.36 \). The backscatter intensities of one source point are scaled to fit the same plot.
The resonances are labeled as $TE_{n,l}$ or $TM_{n,l}$, where $n$ indicates the mode number, and $l$ the number of radial peaks in the angle-averaged internal energy density distribution [21]. Electromagnetic backscatter intensities show an excellent match between MDRs in both beam focus scenarios. The resonance shape, location, and peak spacing in Fig. 5 match with values from [32]. In Fig. 5(a), the peaks correspond to modes $TE_{39,1}$, $TE_{40,1}$, and $TE_{41,1}$ respectively, and the spacing between the peaks satisfies the $\Delta k\alpha = \pi/2m_r \approx 1.15$ condition. Also, in Fig. 5(b), the MDRs peaks from the coated sphere correspond to the modes $TM_{39,1}$, $TM_{40,1}$, $TM_{41,1}$ and $TM_{42,1}$ respectively.

The MDRs of an individual source point do not match the Gaussian beam resonances. However, a total beam created as a superposition of the source points from the surface $\Omega$ synthesizes the original beam with highly matching MDRs. This leads to the conclusion that the presented 3D ASM combined with the VSH expansion synthesizes electromagnetic scattering from multilayered spheres with high accuracy.

### 3.2. Elliptical source distribution

An elliptical surface was used as an example of a source distribution to synthesize a focused linearly polarized incident field using $\lambda/6$ sampling, see Fig. 6. The incident field is compared to the Physical optics simulations at the $yz$-plane with an excellent agreement to less than a $-39$ dB difference in amplitude and less than the 0.1-degree difference in phase. Also, the scattered fields are computed from a $\alpha = 7.8$ mm radius sphere in $xz$-plane with 100 dielectric layers with linearly varying permittivity $\varepsilon_r \in [1-i0.001, 3-i0.01]$ from the surface to the center.

Base vectors for elliptical surfaces are derived from the Eqs. (1)–(4) with the parametrization

$$\Omega = \begin{cases} \phi(\theta, \phi) = (a_x \sin \theta \cos \phi - x_0)e_x + (b_y \sin \theta \sin \phi - y_0)e_y - (c_z \cos \theta + z_0)e_z \end{cases}$$

$$\theta \in [\pi/6, 2\pi/3], \ \phi \in [-\pi/6, \pi/6]$$

(21)

with axial scaling factors $a_x = 0.6, \ b_y = 1.5, \ c_z = 0.8$ and an unscaled radius $r = 3$. The origin of the ellipsoid is shift $(x_0, y_0, z_0) = (3, 0, -0.5)$ compared to the sphere.
Figure 7 illustrate the amplitude and phase of the total field $E_{\text{tot}} = E_{\text{inc}} + E_{\text{scat}}$ on xz-plane where $x, z \in [-5a, 5a]$. Simulations are performed with $500 \times 500$ evaluation points with size parameter of $k\alpha = 13$ and VSH modes of $N = 70$, see Eq. (26) in the Appendix.

4. Conclusions

We propose a method to compute scattering from multilayered spheres illuminated by incident fields that can be modified freely by adjusting the source distribution’s shape, amplitude, phase, and location. The incident field is presented in a vector spherical harmonic (VSH) expansion defined by the beam shape coefficients (BSCs), and the scattered field is obtained by mapping the incident field BSCs with the T-matrix method.

The goal is achieved by computing BSCs with the 3D angular spectrum method (3D ASM), which we derive by adjusting the curved boundary integral method. The proposed method approximates incident field synthesis from an arbitrary surface, considering the wavelength compared to the surface details. Then, the scattered fields are rigorously computed from approximated incident fields with the Mie theory.

Location and orientation information of 3D ASM sources is transformed in a global coordinate system and mapped into the BSCs to preserve spherical symmetry for VSH expansion. As a result, the total incident field is obtained as a superposition of VSH-expanded source points, in which orientation, locations, and complex amplitude can be adjusted. Each source point affects the total source distribution with an essential point in this approach. If the original $E_0$ is a non-physical distribution, it will be filtered to a physical one, which always satisfies Maxwell’s equations. On the other hand, the final form of the more complex source distributions should be verified by simulations.

Simulations verify the proposed method’s incident field synthesis and scattering accuracy. First, we verify the scattering accuracy by comparing the Morphology-dependent resonances (MDRs) from spheres illuminated by the Gaussian beam created from the beam waist by nominal 2D ASM and by more complex electric field distribution with the proposed 3D ASM. The MDRs resonances of the Gaussian beam synthesized by the 3D ASM were in excellent agreement with the reference values, validating the high accuracy on the scattered fields. Hereafter, we demonstrate the method’s practicality by synthesizing an incident field from an elliptical surface and computing scattered fields from a 100-layer sphere.

The novelty of this approach lies in a straightforward simulation algorithm, where the incident field can be defined at any parametrized surface. Furthermore, the parameterized surface can be located inside the computational domain, on the surface, or inside the spherical scatterer without restrictions and source singularities. Unrestricted placement of the source distribution has clear
advantages, especially in the inverse beam design, where the desired beam is defined on the sub-region on the spherical scatterer. Additionally, the synthesized beam can be reradiated from any evaluation surface to another, enabling beam simulation between optical elements with the ability to consistently compute the scattered fields from multilayered spheres.

Appendix

The VSH beam shape coefficients for each $ij$–plane wave of the incident field is defined as [33]

\[
d_{emn} = 4r^2 e_{ij} \cdot \left[ -e_\theta \sin (m\phi) \frac{m}{\sin \theta} P_m^m(\cos \theta) - e_\phi \cos (m\phi) \frac{d}{d\theta} P_m^m(\cos \theta) \right],
\]

\[
d_{omn} = 4r^2 e_{ij} \cdot \left[ e_\theta \cos (m\phi) \frac{m}{\sin \theta} P_m^m(\cos \theta) - e_\phi \sin (m\phi) \frac{d}{d\theta} P_m^m(\cos \theta) \right],
\]

\[
b_{emn} = -4 P^{m+1}_n e_{ij} \cdot \left[ e_\theta \cos (m\phi) \frac{m}{\sin \theta} P_m^m(\cos \theta) - e_\phi \sin (m\phi) \frac{d}{d\theta} P_m^m(\cos \theta) \right],
\]

\[
b_{omn} = -4 P^{m+1}_n e_{ij} \cdot \left[ e_\theta \sin (m\phi) \frac{m}{\sin \theta} P_m^m(\cos \theta) + e_\phi \cos (m\phi) \frac{d}{d\theta} P_m^m(\cos \theta) \right],
\]

where $P_m^m$ is the associated Legendre function of the first kind of degree $n$ and order $m$. Additionally, $\theta, \phi$ are spherical coordinates and $e_\theta, e_\phi$ spherical base vectors of $\mathbf{r}$ in the local base $(e_1, e_2, e_3)$ as in Eq. (19). The scattered electric and magnetic fields from a differential element in the VSH presentation are obtained as

\[
\mathbf{E}(\mathbf{r}; \mathbf{a})_{scat} = (kp)^2 \sum_{m} \sum_{n} D_{mn} \left[ f_{emn} M_{emn}^{(3)}(k \mathbf{r}) + f_{omn} M_{omn}^{(3)}(k \mathbf{r}) \right] + g_{emn} N_{emn}^{(3)}(k \mathbf{r}) + g_{omn} N_{omn}^{(3)}(k \mathbf{r}),
\]

\[
\mathbf{H}(\mathbf{r}; \mathbf{a})_{scat} = -\frac{i(kp)^2}{\eta} \sum_{m} \sum_{n} D_{mn} \left[ g_{emn} M_{emn}^{(3)}(k \mathbf{r}) + g_{omn} M_{omn}^{(3)}(k \mathbf{r}) \right] + f_{emn} N_{emn}^{(3)}(k \mathbf{r}) + f_{omn} N_{omn}^{(3)}(k \mathbf{r}),
\]

where the superscripts $(3)$ present the vector spherical harmonics (outgoing wave) with spherical Hankel function of the first kind $h_1^{(1)}(kr)$ and $\eta = 120\pi$ is the free space impedance. The $f_{emn}, f_{omn}, g_{emn}$ and $g_{omn}$ are vector spherical harmonic coefficient for the scattered field calculated from the T-matrix method as

\[
[f_{emn} f_{omn} g_{emn} g_{omn}]^T = T [a_{emn} a_{omn} B_{emn} B_{omn}]^T
\]

where the T-matrix elements for the multilayered sphere are obtained by the algorithm defined in [34]. The scattered electric and magnetic fields are presented as

\[
\mathbf{E}(\mathbf{r})_{sca} = \frac{1}{4\pi} \int_{\Omega} \mathbf{E}_0(\mathbf{o}) \mathbf{E}(\mathbf{r}; \mathbf{o})_{scat} d\Omega,
\]

\[
\mathbf{H}(\mathbf{r})_{sca} = \frac{1}{4\pi} \int_{\Omega} \mathbf{E}_0(\mathbf{o}) \mathbf{H}(\mathbf{r}; \mathbf{o})_{scat} d\Omega
\]

The required number of the VSH modes ($N_{req}$) for the series to convergence is defined as a function of size parameter $x_i = kr$ and $N_{req} = \max(N_{stop}, |n_i x_i|, |n_i x_{i-1}|) + 15$ when $l = 1, 2, ... L$ and $[22]

\[
N_{stop} = \begin{cases} x_i + 4x_i^{1/3} + 1 & 0.02 \leq x_i < 8 \\ x_i + 4.05x_i^{1/3} + 2 & 8 \leq x_i < 4200 \\ x_i + 4x_i^{1/3} + 2 & 4200 \leq x_i < 20,000, \end{cases}
\]

where $n_i$ is the refractive index of the layer $l$ and $L$ is the number of the layers.

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References