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A simple and robust surface integral method to model light and matter interactions

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We introduce a robust and effective surface integral equation method for modelling light-matter interactions which is simple conceptually and only encompasses the key tasks to obtain the physically important values of the field and its derivative at the surface that are often of interest in micro-photonic applications.

In the frequency domain with time dependence of $\exp(-\mathrm{i}\omega t)$, when an incident electric field is scattered by homogeneous objects in a source-free and homogeneous medium, the scattered and the transmitted electric fields obey

$$\nabla^2 \boldsymbol{E} + k^2 \boldsymbol{E} = \boldsymbol{0}, \tag{1}$$
$$\nabla \cdot \boldsymbol{E} = 0, \tag{2}$$

where $k^2 \equiv \omega^2 \epsilon \mu$ is the wave number, $\epsilon \equiv \epsilon_0 \epsilon_r$ and $\mu \equiv \mu_0 \mu_r$ are, respectively, the permittivity and permeability of the medium or the scatterers.

The key of our method is that, for condition (2), we have proved rigorously that if the electric field is divergence-free at all points on the scatterer surface S which encloses the domain, then the electric field is divergence-free everywhere in the 3D domain.[1,2] Explicitly, $\nabla \cdot \boldsymbol{E}$ on surface S is:

$$\nabla \cdot \boldsymbol{E} = \boldsymbol{n} \cdot \frac{\partial \boldsymbol{E}}{\partial n} - \kappa E_n + \frac{\partial E_{t_1}}{\partial t_1} + \frac{\partial E_{t_2}}{\partial t_2} = 0, \tag{3}$$

where κ is the mean curvature. In (3), $E_n \equiv \boldsymbol{E} \cdot \boldsymbol{n}$ is the normal component of $\boldsymbol{E}$, and $E_{t_1} \equiv \boldsymbol{E} \cdot \boldsymbol{t}_1$ and $E_{t_2} \equiv \boldsymbol{E} \cdot \boldsymbol{t}_2$ are the tangential components of $\boldsymbol{E}$ along the two mutually perpendicular tangential unit vectors $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$. The tangential derivatives are defined by $\partial(\cdot)/\partial t_j \equiv \boldsymbol{t}_j \cdot \nabla(\cdot)$ for $j = 1, 2$, respectively. Note that (3) is valid for both the scattered and transmitted fields. Also, we can write the non-singular surface integral representation[3,4] for each Cartesian component of the electric field in (1). Together with the boundary conditions that the tangential components of the electric and magnetic fields are continuous cross the boundary, we then develop a simple and robust surface integral equation (SIE) method to model the interactions between light and matter.

The proposed SIE method has the following advantages: 1) It is conceptually simple, and it focuses on solving directly for physically important quantities namely, the electric field and its normal derivative; 2) It only requires a surface solver for the scalar Helmholtz equation; 3) Together with Fourier transformations, this method can solve time domain scattering problems straightforwardly; 4) The electric field on, near, inside and far away from dielectric scatterers can be obtained easily; 5) It is stable in full wavelength, so that this method is capable to solve a broad range of phenomena from electrostatic polarization to wave optics and geometric optics, which makes it most suitable to investigate multi-scale problems.

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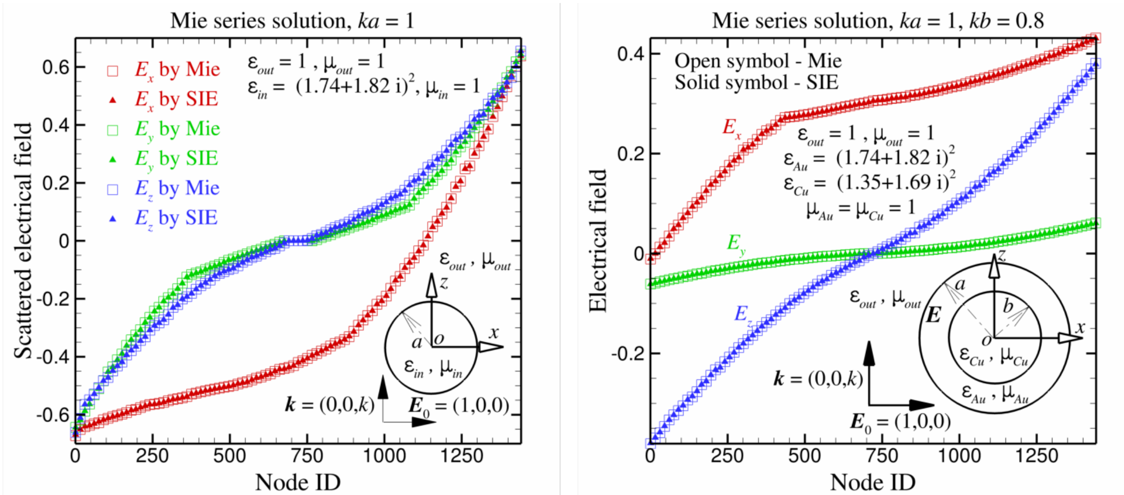

(a) (b)

Figure 1. (a) Scattered electric field (real part) on the surface of a Au sphere with radius of 50 nm in an incident field: $\boldsymbol{E}^{\text{inc}} = (1, 0, 0) \exp(\text{i}kz)$ which wavelength is $\lambda = 314$ nm as $ka = 1$. (b) The transmitted electric field on the outer boundary of the Au shell when the same incident field as in (a) is scattered by a multi-layer sphere with Au shell which radius is $a = 50$ nm and Cu core which radius is $b = 40$ nm.

To demonstrate our method, in Fig. 1a, we illustrate an example to deal with an incident light, which is treated as a plane wave as $\boldsymbol{E}^{\text{inc}} = (1, 0, 0) \exp(\text{i}kz)$, scattered by an Au sphere in air. The wavelength of the incident wave is chosen as $\lambda = 314$ nm and the Au sphere radius as $a = 50$ nm which leads to $ka = 1$. As shown in Fig. 1a, the scattered electric field calculated by our field-only surface integral method are in good agreement with the well-known Mie series solutions.[5] We then extended the complexity of the problem by embedding a copper (Cu) core with radius as $b = 40$ nm in the Au sphere to make the scatterer become a core-shell or multi-layer structure. The transmitted electric field on the outer boundary of the Au shell is presented in Fig. 1b when this core-shell sphere is hit by the same plane wave. We can see that the numerical results obtained by our method agree well with the Mie series.[5] Note that in Fig. 1, the data have been organised with the nodes renumbered in increasing order of the field components for visual clarity, and the dielectric constants of Au and Cu are calculated by the Brendel-Bormann model.[6]

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