

Coupled Solution of Volume Integral and Hydrodynamic Equations to Analyze Electromagnetic Scattering From Composite Nanostructures

Doolos Aibek Uulu¹, *Student Member, IEEE*, Rui Chen¹, *Member, IEEE*, Liang Chen¹, *Senior Member, IEEE*, Ping Li², *Senior Member, IEEE*, and Hakan Bagci¹, *Senior Member, IEEE*

Abstract—A coupled system of volume integral and hydrodynamic equations is solved to analyze electromagnetic scattering from nanostructures consisting of metallic and dielectric parts. In the metallic part, the hydrodynamic equation relates the free electron polarization current to the electric flux and effectively “updates” the constitutive relationship to enable the modeling of nonlocality. In the metallic and dielectric parts, the volume integral equation relates the electric flux and the free electron polarization current to the scattered electric field. Unknown electric flux and free electron polarization current are expanded using Schaubert–Wilton–Glisson (SWG) basis functions. Inserting these expansions into the coupled system of the volume integral and hydrodynamic equations and using Galerkin testing yield a matrix system in unknown expansion coefficients. An efficient two-level iterative solver is proposed to solve this matrix system. This approach “inverts” the discretized hydrodynamic equation for the coefficients of the free electron polarization current and substitutes the result in the discretized volume integral equation. Outer iterations solve this reduced matrix system while the inner iterations invert the discretized hydrodynamic equation at every iteration of the outer iterations. Numerical experiments are carried out to demonstrate the accuracy, the efficiency, and the applicability of the proposed method.

Index Terms—Electromagnetic scattering, hydrodynamic equation, nonlocal effects, plasmonic nanostructures, volume integral equation.

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Doolos Aibek Uulu, Liang Chen, and Hakan Bagci are with the Electrical and Computer Engineering Program, Computer, Electrical, and Mathematical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia (e-mail: doolos.aibekuulu@kaust.edu.sa; liang.chen@kaust.edu.sa; hakan.bagci@kaust.edu.sa).

Rui Chen was with the Electrical and Computer Engineering Program, Computer, Electrical, and Mathematical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia. He is now with the Department of Communication Engineering, Nanjing University of Science and Technology, Nanjing 210094, China (e-mail: rui.chen@kaust.edu.sa).

Ping Li is with the Key Laboratory of Ministry of Education of Design and Electromagnetic Compatibility of High-Speed Electronic Systems, Shanghai Jiao Tong University, Shanghai 200240, China (e-mail: ping.li@sjtu.edu.cn).

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I. INTRODUCTION

IN RECENT years, with the dramatic advances in fabrication technologies, the use of plasmonic nanostructures to manipulate high-frequency electromagnetic fields has become more prevalent than ever [1], [2]. Often, metals are used as the building blocks of these nanostructures since they support surface plasmon modes at optical frequencies. These modes localize the electromagnetic fields in the proximity of the nanostructure and significantly enhance those scattered from it in the far-field region. This has enabled the use of metallic nanostructures as nanoantennas [3], resonators [4], waveguides [5], couplers [6], and sensors [7].

Depending on the frequency, interaction of electromagnetic fields with metals can be accounted for using various models and equations under certain assumptions and approximations. At microwave frequencies, free electrons in a metal have high mobility, which leads to large conductivity and small skin depth (compared with the size of the structure) [8]. Therefore, an electric current, which is confined to the surface of the metal, is used to represent the electromagnetic field interactions on the metal. At optical frequencies, the free electron mobility decreases. As a result, there is a time delay in the response of the electrons to the electromagnetic excitation [9]. To account for this frequency dispersion effect, the classical Drude model [10] is used to represent the permittivity of the metal. Furthermore, at the optical frequencies, the skin depth is usually comparable to the size of a typical nanostructure and the metals are modeled as “penetrable” materials and volume electric currents are used to represent the electromagnetic field interactions on or inside them.

When the frequency is further increased into the ultraviolet part of the spectrum, spatial dispersion appears in the response of the free electrons to the electromagnetic excitation. Effectively, the permittivity becomes nonlocal, i.e., it depends not only on the observation point but also on the source point in space [11]. This spatial dispersion effect is due to the fact that at this frequency regime, a free electron exhibits quantum behavior [12], and the interactions of the electromagnetic fields with the electrons should ideally be modeled using full quantum mechanics simulation methods (e.g., density functional theory [13]). However, the computational cost of

these methods is very high, and, therefore, they can only be used when the structure is very small, i.e., only a few nanometers in size [14]. This makes them unsuitable for full-scale simulations of plasmonic nanostructures in real-life scenarios.

This bottleneck can be addressed using a hydrodynamic equation to model the mechanical motion of the free electrons [11]. This equation assumes that the electrons can collectively be accounted for as a moving fluid of charges driven by the electromagnetic fields in the medium. Naturally, these moving charges (termed as the free electron polarization current in the rest of the text) generate electromagnetic fields. This interaction between the free electrons and the electromagnetic fields can be described by a coupled system of the Maxwell and hydrodynamic equations [15], [16], [17], [18], [19]. This system of coupled equations can account for the nonlocality/spatial dispersion and its numerical solution is not as costly as that of the full quantum mechanics simulation methods.

Several methods have been developed to numerically solve the coupled system of the Maxwell and hydrodynamic equations [15], [16], [17], [18], [19]. A majority of these methods are differential equation solvers, e.g., finite element method [16], finite-difference time-domain method [17], and discontinuous Galerkin method [18], [19]. These solvers, just like their traditional versions, which are developed to solve only the Maxwell equations, suffer from several well-known shortcomings that might limit their accuracy and efficiency (see, for example, [20] for details).

Surface integral equation solvers do not suffer from these shortcomings (see, for example, again [20] for details), and indeed, they have been extended to analyze scattering from metallic objects in which the motion of electrons is described by the hydrodynamic equation [15]. However, this method requires the derivation of a new Green function for every type of boundary condition and their combination enforced by the hydrodynamic equation (for example, boundary conditions for the free electron polarization current on metal–metal or metal–dielectric interfaces are different). In addition, this solver is applicable only when the scatterer has homogeneous or piecewise homogeneous material properties.

In this work, these shortcomings are avoided by switching to a volume integral equation formulation. The proposed scheme represents the scattered electromagnetic field in the form of a (volumetric) convolution between the background medium’s Green function and the electric flux (induced in the metallic and dielectric parts of the scatterer) and the free electron polarization current (induced in the metallic part). In both the metallic and dielectric parts, the volume integral equation, which relates the electric flux and the free electron polarization current to the scattered electric field, is enforced. In the metallic part, the hydrodynamic equation, which relates the free electron polarization current to the electric flux, is enforced. To numerically solve this coupled system of equations, first the scatterer is discretized into a mesh of tetrahedrons. The electric flux and the free electron polarization current are expanded using a combination of “full” and “half” Schaubert–Wilton–Glisson (SWG) basis

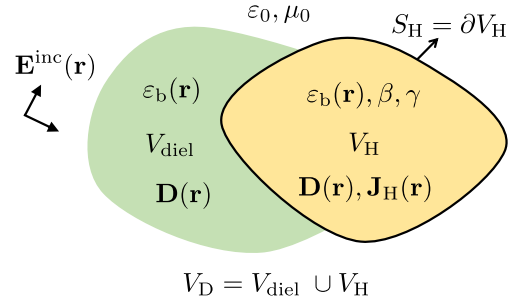


Fig. 1. Description of the scattering problem.

functions [21] defined on these tetrahedrons. Inserting these expansions into the coupled system of the volume integral and the hydrodynamic equations and applying Galerkin testing yield a matrix system in unknown expansion coefficients. The boundary condition for the normal component of the free electron polarization current (which should be set to zero on a metal–dielectric interface) is enforced by excluding the half SWG functions, which are defined on the tetrahedrons that have a face on the metal–dielectric interface, from the expansion of the free electron polarization current.

An efficient two-level iterative solver is developed to solve the matrix system resulting from this discretization. This solver “inverts” the discretized hydrodynamic equation for the coefficients of the free electron polarization current and substitutes the result in the discretized volume integral equation. Outer iterations solve this reduced matrix system, while the inner iterations invert the discretized hydrodynamic equation at every iteration of the outer iterations. Note that a preliminary version of the method proposed in this work has been described in [22] as a conference contribution.

The remainder of this article is organized as follows. Sections II–A–II–C describe the formulation of the coupled system of the volume integral and the hydrodynamic equations, its discretization, and the two-level iterative solution, respectively. Section II–D explains how the mesh element size is selected and provides several comments on possible extensions of the proposed method and its applications. Section III presents the numerical results that demonstrate the accuracy, the efficiency, and the applicability of the proposed scheme. Finally, Section IV summarizes this work and outlines future research directions.

II. FORMULATION

A. Coupled System of the Volume Integral and the Hydrodynamic Equations

Let V_D represent a composite scatterer that consists of dielectric and metallic parts (Fig. 1). V_{diel} and V_H represent these parts, respectively. Both V_{diel} and V_H are non-magnetic but their relative permittivity (for bound electron polarization) as denoted by $\epsilon_b(\mathbf{r})$ can be inhomogeneous. The boundary surface of V_H is represented by S_H . The scatterer resides in an unbounded homogeneous background medium with permittivity ϵ_0 and permeability μ_0 . The electric field of the excitation is denoted by $\mathbf{E}^{\text{inc}}(\mathbf{r})$ and its frequency is denoted by ω .

Upon this excitation, equivalent volumetric electric current $\mathbf{J}(\mathbf{r})$ is induced in V_D and this current generates the scattered electric field $\mathbf{E}^{\text{sca}}(\mathbf{r})$. The incident electric field $\mathbf{E}^{\text{inc}}(\mathbf{r})$, the scattered electric field $\mathbf{E}^{\text{sca}}(\mathbf{r})$, and the total electric field $\mathbf{E}(\mathbf{r})$ satisfy the fundamental field relationship.

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}^{\text{inc}}(\mathbf{r}) + \mathbf{E}^{\text{sca}}(\mathbf{r}). \quad (1)$$

Using the volume equivalence principle [20], $\mathbf{J}(\mathbf{r})$ is expressed in terms of $\mathbf{E}(\mathbf{r})$ and the electric flux $\mathbf{D}(\mathbf{r})$ as follows:

$$\mathbf{J}(\mathbf{r}) = j\omega\mathbf{D}(\mathbf{r}) - j\omega\varepsilon_0\mathbf{E}(\mathbf{r}), \quad \mathbf{r} \in V_D \quad (2)$$

and $\mathbf{E}^{\text{sca}}(\mathbf{r})$ is expressed as follows:

$$\mathbf{E}^{\text{sca}}(\mathbf{r}) = \mathcal{L}_{V_D}[\mathbf{J}](\mathbf{r}). \quad (3)$$

Here, $\mathcal{L}_V[\mathbf{X}](\mathbf{r})$ is the volume integral operator given by the following equation:

$$\begin{aligned} \mathcal{L}_V[\mathbf{X}](\mathbf{r}) = & -j\omega\mu_0 \int_V \mathbf{X}(\mathbf{r}')G(\mathbf{r}, \mathbf{r}')dv' \\ & + \frac{1}{j\omega\varepsilon_0} \int_V \nabla\nabla \cdot [\mathbf{X}(\mathbf{r}')G(\mathbf{r}, \mathbf{r}')]dv' \end{aligned}$$

where $G(\mathbf{r}, \mathbf{r}') = \exp(-jk_0R)/(4\pi R)$ is the Green function, $k_0 = \omega\sqrt{\mu_0\varepsilon_0}$ is the wavenumber in the background medium, and $R = |\mathbf{r} - \mathbf{r}'|$ denotes the distance between the observation point \mathbf{r} and the source point \mathbf{r}' .

The motion of the free electrons in V_H is accounted for using a nonlocal hydrodynamic equation. Let $\mathbf{J}_H(\mathbf{r})$ represent the polarization current associated with these free electrons. Then, $\mathbf{J}_H(\mathbf{r})$ is expressed in terms of $\mathbf{E}(\mathbf{r})$ and $\mathbf{D}(\mathbf{r})$ as [15]

$$\mathbf{J}_H(\mathbf{r}) = j\omega\mathbf{D}(\mathbf{r}) - j\omega\varepsilon_0\varepsilon_b(\mathbf{r})\mathbf{E}(\mathbf{r}), \quad \mathbf{r} \in V_H. \quad (4)$$

In addition, $\mathbf{J}_H(\mathbf{r})$ is “driven” by $\mathbf{E}(\mathbf{r})$. This relationship is described by the nonlocal hydrodynamic Drude equation as [11]

$$\begin{aligned} \beta^2\nabla[\nabla \cdot \mathbf{J}_H(\mathbf{r})] + \omega(\omega - j\gamma)\mathbf{J}_H(\mathbf{r}) \\ = -j\omega\omega_p^2\varepsilon_0\mathbf{E}(\mathbf{r}), \quad \mathbf{r} \in V_H. \end{aligned} \quad (5)$$

Here, ω_p is the plasma frequency, $\beta^2 = 0.6v_F^2$, v_F is the Fermi velocity, and γ is a damping constant. The hydrodynamic (5) has to be complemented by a boundary condition on the boundary surface of V_H [as denoted by S_H (Fig. 1)] [11]

$$\hat{\mathbf{n}}(\mathbf{r}) \cdot \mathbf{J}_H(\mathbf{r}) = 0, \quad \mathbf{r} \in S_H. \quad (6)$$

Here, $\hat{\mathbf{n}}(\mathbf{r})$ is the outward pointing unit normal vector on S_H . This boundary condition ensures that the normal component of $\mathbf{J}_H(\mathbf{r})$ vanishes on S_H (i.e., free electrons do not flow from the metallic part into the dielectric part or the background medium). Note that the hydrodynamic (5) together with the boundary condition (6) introduces an electromagnetic wave solution with a longitudinal electric field in V_H in addition to the one with a transverse electric field [11].

The proposed scheme defines $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ as unknowns. To eliminate $\mathbf{E}(\mathbf{r})$, $\mathbf{E}(\mathbf{r})$ from (4) is inserted into (2). This yields an expression for $\mathbf{J}(\mathbf{r})$ in terms of $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ as follows:

$$\mathbf{J}(\mathbf{r}) = j\omega\kappa(\mathbf{r})\mathbf{D}(\mathbf{r}) + \frac{\mathbf{J}_H(\mathbf{r})}{\varepsilon_b(\mathbf{r})}, \quad \mathbf{r} \in V_H \quad (7)$$

where $\kappa(\mathbf{r}) = 1 - 1/\varepsilon_b(\mathbf{r})$. Substituting (7) into (3) and inserting the resulting equation and $\mathbf{E}(\mathbf{r})$ from (4) into (1) yield the volume integral equation in unknowns $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ as follows:

$$\begin{aligned} \mathbf{E}^{\text{inc}}(\mathbf{r}) = & \frac{\mathbf{D}(\mathbf{r})}{\varepsilon_0\varepsilon_b(\mathbf{r})} - j\omega\mathcal{L}_{V_D}[\kappa\mathbf{D}](\mathbf{r}) \\ & - \frac{\mathbf{J}_H(\mathbf{r})}{j\omega\varepsilon_0\varepsilon_b(\mathbf{r})} - \mathcal{L}_{V_H}\left[\frac{\mathbf{J}_H}{\varepsilon_b}\right](\mathbf{r}), \quad \mathbf{r} \in V_D. \end{aligned} \quad (8)$$

Similarly, the hydrodynamic (5) should be expressed in only $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$. Inserting $\mathbf{E}(\mathbf{r})$ from (4) into (5) yields

$$\begin{aligned} \beta^2\nabla[\nabla \cdot \mathbf{J}_H(\mathbf{r})] + \left[\omega(\omega - j\gamma) - \frac{\omega_p^2}{\varepsilon_b(\mathbf{r})} \right] \mathbf{J}_H(\mathbf{r}) \\ = -j\omega\omega_p^2 \frac{\mathbf{D}(\mathbf{r})}{\varepsilon_b(\mathbf{r})}, \quad \mathbf{r} \in V_H. \end{aligned} \quad (9)$$

Equations (8) and (9) are the final form of the coupled system of the volume integral and the hydrodynamic equations in unknowns $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$. This system is discretized using the scheme described in Section II-B. Note that this discretization scheme ensures that the boundary condition (6) is enforced correctly.

B. Discretization

To numerically solve the coupled system of (8) and (9), first, V_D is discretized into a mesh of tetrahedrons. Then, the unknowns $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ are expanded as follows:

$$\begin{aligned} \mathbf{D}(\mathbf{r}) = \sum_{n=1}^{N_D} \{\mathbf{I}_D\}_n \mathbf{f}_n^D(\mathbf{r}), \quad \mathbf{r} \in V_D \\ \mathbf{J}_H(\mathbf{r}) = \sum_{n=1}^{N_H} \{\mathbf{I}_H\}_n \mathbf{f}_n^H(\mathbf{r}), \quad \mathbf{r} \in V_H. \end{aligned} \quad (10)$$

Here, $\{\mathbf{I}_D\}_n$ and $\{\mathbf{I}_H\}_n$ are the unknown coefficients, and $\mathbf{f}_n^D(\mathbf{r})$ and $\mathbf{f}_n^H(\mathbf{r})$ are the basis functions constructed using the SWG functions defined on the triangles of the tetrahedral mesh [21]. The SWG basis function associated with triangle n is defined as follows:

$$\mathbf{f}_n(\mathbf{r}) = \begin{cases} \mathbf{f}_n^+(\mathbf{r}) = \frac{|S_n|}{3|V_n^+|}(\mathbf{r} - \mathbf{r}_n^+), & \mathbf{r} \in V_n^+ \\ \mathbf{f}_n^-(\mathbf{r}) = -\frac{|S_n|}{3|V_n^-|}(\mathbf{r} - \mathbf{r}_n^-), & \mathbf{r} \in V_n^- \\ 0, & \text{elsewhere.} \end{cases} \quad (11)$$

Here, V_n^+ and V_n^- are the tetrahedrons “touching” triangle n on its two sides, \mathbf{r}_n^\pm are the corners of V_n^\pm that are not on S_n (i.e., free nodes), $|S_n|$ is the area of S_n , and $|V_n^\pm|$ are the volumes of V_n^\pm .

The basis set $\mathbf{f}_n^D(\mathbf{r})$ includes “full” SWG basis functions as defined by (11) on every pair of tetrahedrons in V_D and “half” SWG basis functions defined by $\mathbf{f}_n^+(\mathbf{r})$ of (11) in single tetrahedrons that have their S_n on the surface of the scatterer. The use of full SWG functions enforces the continuity of the normal component of $\mathbf{D}(\mathbf{r})$ across any pair of tetrahedrons in V_D (even when $\varepsilon_b(\mathbf{r})$ in V_n^+ and V_n^- are different). The inclusion of half SWG functions ensures that the normal

component of $\mathbf{D}(\mathbf{r})$ on the surface of the scatterer is accounted for. N_D in (10) is the total number of full and half SWG basis functions used in the expansion of $\mathbf{D}(\mathbf{r})$ in V_D .

The basis set $\mathbf{f}_n^H(\mathbf{r})$ consists of only the full basis functions as defined by (11) on every pair of tetrahedrons in V_H and does not include the half SWG basis functions defined in single tetrahedrons that have their S_n on S_H (metal-dielectric interface). Note that $\mathbf{J}_H(\mathbf{r})$ does not flow from the metallic part into the dielectric part or the background medium and its normal component on S_H is zero as described by the boundary condition in (6). Exclusion of the half SWG basis functions from $\mathbf{f}_n^H(\mathbf{r})$ ensures that this boundary condition is correctly enforced. N_H in (10) is the total number of full SWG basis functions used in the expansion of $\mathbf{J}_H(\mathbf{r})$ in V_H .

Inserting the expansions (10) into (8) and (9) and Galerkin testing the resulting equations using $\mathbf{f}_m^D(\mathbf{r})$, $m = 1, 2, \dots, N_D$ and $\mathbf{f}_m^H(\mathbf{r})$, $m = 1, 2, \dots, N_H$ yield a coupled matrix system of dimension $(N_D + N_H) \times (N_D + N_H)$ as follows:

$$\underbrace{\begin{bmatrix} \mathbf{Z}_{DD} & \mathbf{Z}_{DH} \\ \mathbf{Z}_{HD} & \mathbf{Z}_{HH} \end{bmatrix}}_{\mathbf{Z}} \underbrace{\begin{bmatrix} \mathbf{I}_D \\ \mathbf{I}_H \end{bmatrix}}_{\mathbf{I}} = \underbrace{\begin{bmatrix} \mathbf{V}^{\text{inc}} \\ \mathbf{0} \end{bmatrix}}_{\mathbf{V}}. \quad (12)$$

In (12), the entries of the block matrices \mathbf{Z}_{DD} of dimension $N_D \times N_D$, \mathbf{Z}_{DH} of dimension $N_D \times N_H$, \mathbf{Z}_{HD} of dimension $N_H \times N_D$, \mathbf{Z}_{HH} of dimension $N_H \times N_H$, and the tested incident field vector \mathbf{V}^{inc} of dimension N_D are given by the following equations:

$$\{\mathbf{Z}_{DD}\}_{mn} = \frac{1}{\varepsilon_0} \left\langle \mathbf{f}_m^D(\mathbf{r}), \frac{\mathbf{f}_n^D(\mathbf{r})}{\varepsilon_b(\mathbf{r})} \right\rangle - j\omega \left\langle \mathbf{f}_m^D(\mathbf{r}), \mathcal{L}_{V_D}[\kappa \mathbf{f}_n^D](\mathbf{r}) \right\rangle \quad (13)$$

$$\{\mathbf{Z}_{DH}\}_{mn} = -\frac{1}{j\omega\varepsilon_0} \left\langle \mathbf{f}_m^D(\mathbf{r}), \frac{\mathbf{f}_n^H(\mathbf{r})}{\varepsilon_b(\mathbf{r})} \right\rangle - \left\langle \mathbf{f}_m^D(\mathbf{r}), \mathcal{L}_{V_H} \left[\frac{\mathbf{f}_n^H}{\varepsilon_b} \right](\mathbf{r}) \right\rangle \quad (14)$$

$$\{\mathbf{Z}_{HD}\}_{mn} = j\omega\omega_p^2 \left\langle \mathbf{f}_m^H(\mathbf{r}), \frac{\mathbf{f}_n^D(\mathbf{r})}{\varepsilon_b(\mathbf{r})} \right\rangle \quad (15)$$

$$\{\mathbf{Z}_{HH}\}_{mn} = \beta^2 \left\langle \mathbf{f}_m^H(\mathbf{r}), \nabla[\nabla \cdot \mathbf{f}_n^H(\mathbf{r})] \right\rangle + \omega(\omega - j\gamma) \times \left\langle \mathbf{f}_m^H(\mathbf{r}), \frac{\mathbf{f}_n^H(\mathbf{r})}{\varepsilon_b(\mathbf{r})} \right\rangle \quad (16)$$

$$\{\mathbf{V}^{\text{inc}}\}_m = \left\langle \mathbf{f}_m^D(\mathbf{r}), \mathbf{E}^{\text{inc}}(\mathbf{r}) \right\rangle \quad (17)$$

respectively. Here, the inner product between vector functions $\mathbf{a}(\mathbf{r})$ and $\mathbf{b}(\mathbf{r})$ is defined as follows:

$$\langle \mathbf{a}(\mathbf{r}), \mathbf{b}(\mathbf{r}) \rangle = \int_{V_a} \mathbf{a}(\mathbf{r}) \cdot \mathbf{b}(\mathbf{r}) dv \quad (18)$$

where V_a is the support of $\mathbf{a}(\mathbf{r})$. Since $\mathcal{L}_{V_D}(\mathbf{X})[\mathbf{r}]$ and $\mathcal{L}_{V_H}(\mathbf{X})[\mathbf{r}]$ are ‘‘global’’ operators, one can see from (13) and (14) that \mathbf{Z}_{DD} and \mathbf{Z}_{DH} are dense matrix blocks. On the other hand, since $\mathbf{f}_n^D(\mathbf{r})$ and $\mathbf{f}_n^H(\mathbf{r})$ have ‘‘local’’ supports (two tetrahedrons for a full SWG function and one tetrahedron for a half SWG function), one can see from (15) and (16) that \mathbf{Z}_{HD} and \mathbf{Z}_{HH} are sparse matrix blocks (the maximum number of nonzero entries in one row of these blocks is seven). Note that the detailed expressions for the matrix entries in (13)–(16) and the vector entries in (17) are provided in the Appendix.

C. Solution of the Matrix equation

To take advantage of the sparsity of \mathbf{Z}_{HD} and \mathbf{Z}_{HH} directly, the coupled matrix system (12) is solved iteratively for the unknown coefficient vectors \mathbf{I}_D and \mathbf{I}_H . Two approaches can be used for this purpose.

1) *Single-Level Iterative Solver*: The coupled system (12) is iteratively solved as a whole using a transpose-free quasi-minimal residual (TFQMR) scheme [23]. The computational cost of matrix–vector multiplication $\mathbf{Z}\tilde{\mathbf{I}}$ required at every iteration of TFQMR scales as $\mathcal{O}(N_D^2) + \mathcal{O}(N_D N_H) + \mathcal{O}(N_H) + \mathcal{O}(N_H)$. The four terms in this expression represent the computational cost of multiplying matrix blocks \mathbf{Z}_{DD} , \mathbf{Z}_{DH} , \mathbf{Z}_{HD} , and \mathbf{Z}_{HH} with the relevant part of $\tilde{\mathbf{I}}$, respectively. Then, the overall computational cost of this single-level iterative solver scales as follows:

$$\mathcal{O}(N_{\text{it}} N_D^2) + \mathcal{O}(N_{\text{it}} N_D N_H) + \mathcal{O}(N_{\text{it}} N_H) + \mathcal{O}(N_{\text{it}} N_H) \quad (19)$$

where N_{it} is the number of iterations required for the relative residual error to converge to a user-defined value.

2) *Two-Level Iterative Solver*: In this approach, before an iterative solver is used, the coupled system (12) is first reduced into a smaller matrix system. This is done by inverting the second row of (12) for \mathbf{I}_H , i.e., $\mathbf{I}_H = -\mathbf{Z}_{HH}^{-1} \mathbf{Z}_{HD} \mathbf{I}_D$, and inserting this expression into the first row. This yields a smaller matrix system of dimension $N_D \times N_D$ in unknown \mathbf{I}_D as follows:

$$(\mathbf{Z}_{DD} - \mathbf{Z}_{DH} \mathbf{Z}_{HH}^{-1} \mathbf{Z}_{HD}) \mathbf{I}_D = \mathbf{V}^{\text{inc}}. \quad (20)$$

Then, TFQMR is used to solve (20) for \mathbf{I}_D . Matrix–vector multiplication $(\mathbf{Z}_{DD} - \mathbf{Z}_{DH} \mathbf{Z}_{HH}^{-1} \mathbf{Z}_{HD}) \tilde{\mathbf{I}}_D$ required at every iteration of TFQMR is carried out as described below.

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- Step 1*: Compute the first term $\mathbf{Z}_{DD} \tilde{\mathbf{I}}_D$.
Step 2: Compute the second term $\mathbf{Z}_{DH} \mathbf{Z}_{HH}^{-1} \mathbf{Z}_{HD} \tilde{\mathbf{I}}_D$ in three steps as
Step 2.1: Compute $\mathbf{y} = \mathbf{Z}_{HD} \tilde{\mathbf{I}}_D$.
Step 2.2: Compute $\mathbf{x} = \mathbf{Z}_{HH}^{-1} \mathbf{y}$ by solving $\mathbf{y} = \mathbf{Z}_{HH} \mathbf{x}$ for \mathbf{x} . This is done iteratively using TFQMR.
Step 2.3: Compute $\mathbf{Z}_{DH} \mathbf{x}$.
Step 3: Subtract the result of *Step 2.3* from that of *Step 1*.
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Computational costs of *Step 1*, *Step 2.1*, *Step 2.2*, and *Step 2.3* scale as $\mathcal{O}(N_D^2)$, $\mathcal{O}(N_H)$, $\mathcal{O}(N_{\text{it}}^{\text{in}} N_H)$, and $\mathcal{O}(N_D N_H)$, respectively. Here, $N_{\text{it}}^{\text{in}}$ is the number of iterations required for the relative residual error to converge to a user defined value during the solution of the matrix equation $\mathbf{y} = \mathbf{Z}_{HH} \mathbf{x}$ at *Step 2.2* (i.e., inner iterations). Then, the overall computational cost of this two-level iterative solver scales as follows:

$$\mathcal{O}(N_{\text{it}}^{\text{out}} N_D^2) + \mathcal{O}(N_{\text{it}}^{\text{out}} N_H) + \mathcal{O}(N_{\text{it}}^{\text{out}} N_{\text{it}}^{\text{in}} N_H) + \mathcal{O}(N_{\text{it}}^{\text{out}} N_D N_H) \quad (21)$$

where $N_{\text{it}}^{\text{out}}$ is the number of iterations required for the relative residual error to converge to a user defined value during the solution of the matrix (20) (i.e., outer iterations).

Comparing (21) to (19), one can see that the single-level iterative solver would certainly be faster than the two-level

iterative solver for $N_{it} \leq N_{it}^{out}$. However, numerical results presented in Section III-A show that N_{it}^{out} is much smaller than N_{it} and N_{it}^{in} is small, and therefore the two-level iterative solver is significantly faster than the single-level iterative solver. The difference between N_{it} and N_{it}^{out} can be explained by the fact that the dimension of (20) is almost half of that of (12) and inserting $\mathbf{I}_H = -\mathbf{Z}_{HH}^{-1}\mathbf{Z}_{HD}\mathbf{I}_D$ into the first row of (12) [to obtain (20)] effectively takes care of the scaling difference between the volume integral and the hydrodynamic equations.

Note that for both the approaches, the computational cost of matrix–vector multiplications $\mathbf{Z}_{DD}\tilde{\mathbf{I}}_D$ and $\mathbf{Z}_{DH}\tilde{\mathbf{I}}_H$ can be reduced using the fast multipole method [24], [25], [26], [27] and its multilevel versions [28], [29], [30], [31] as well as other matrix compression schemes like those described and referred to in [32], [33], [34], and [35]. But this does not change the conclusions of the above comparison since the difference in the computational cost of the two iterative solvers is mainly due to the difference in the number of iterations.

D. Comments

A metallic medium that is described by the hydrodynamic (5) supports the propagation of electromagnetic waves with electric fields along the transverse and longitudinal directions [11]. Let the (complex) wavenumbers associated with these electromagnetic waves be denoted by $k_T(\mathbf{r})$ and $k_L(\mathbf{r})$, respectively. The expressions of $k_T(\mathbf{r})$ and $k_L(\mathbf{r})$ are given by [11]

$$\begin{aligned} k_T(\mathbf{r}) &= k_0 \sqrt{\varepsilon_b(\mathbf{r}) - \frac{\omega_p^2}{\omega^2 - j\omega\gamma}} \\ k_L(\mathbf{r}) &= \frac{1}{\beta} \sqrt{\omega^2 - j\omega\gamma - \frac{\omega_p^2}{\varepsilon_b(\mathbf{r})}}. \end{aligned} \quad (22)$$

For example, for gold, $\varepsilon_b(\mathbf{r}) = 1$, $\omega_p = 1.20 \times 10^{16} \text{ s}^{-1}$, $\beta = 1.07 \times 10^6 \text{ m/s}$, and $\gamma = 1.36 \times 10^{14} \text{ s}^{-1}$ [36], [37]. Fig. 2 shows the plots of the values of $k_T(\mathbf{r})$ and $k_L(\mathbf{r})$ computed for gold in the frequency range $\omega \in [0.5\omega_p, 1.5\omega_p]$. Note that during the computation of square roots in (22), the positive imaginary part of the result is selected to avoid a nonphysical growing wave. The figure clearly shows that in this frequency range, both the real and imaginary parts of $k_L(\mathbf{r})$ are significantly larger than those of $k_T(\mathbf{r})$, respectively. This means that to accurately capture the behavior of the electromagnetic fields in V_H (inside the metallic part), the mesh of tetrahedrons must resolve the wavelength associated with $k_L(\mathbf{r})$. Note that within the frequency range considered here, since k_0 is significantly smaller than both $k_L(\mathbf{r})$ and $k_T(\mathbf{r})$, the mesh in $V_{diel} = V_D - V_H$ (inside the dielectric part) can ideally be coarser than the one in V_H . But since these two volumes share a surface and a conformal discretization is used, the mesh in V_{diel} is denser than what it would ideally be. This unnecessary computational overhead can be alleviated by switching to a nonconformal discretization scheme, such as the one described in [38] and [39]. Development of such a scheme is underway.

Several comments about the possible extensions of the proposed method are in order.

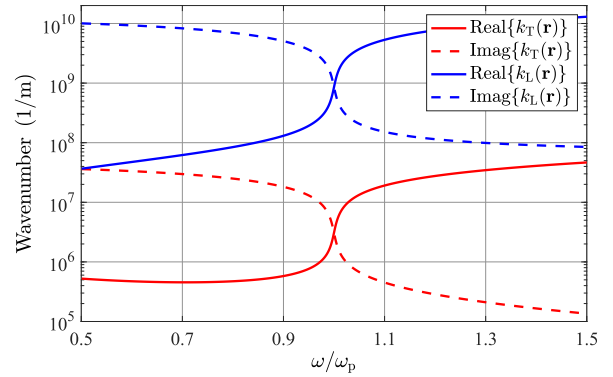


Fig. 2. Wavenumbers of the electromagnetic waves with the transverse and longitudinal electric fields, $k_T(\mathbf{r})$ and $k_L(\mathbf{r})$, versus ω/ω_p .

- 1) The formulation in Section II-A assumes that the scatterer includes only one type of homogeneous metallic structure (described by a set of hydrodynamic equation parameters γ , β , and ω_p). The formulation can easily account for additional metal types described by assigning different values to γ , β , and ω_p in relevant matrix entries as long as the structures made of different metals do not touch each other. This limitation stems from the fact that the boundary condition (6) is not valid on metal–metal interfaces and therefore the discretization scheme described in Section II-B is not applicable anymore. Development of a formulation that removes this limitation and allows for modeling of metal–metal interfaces is currently underway.
- 2) In [40], the nonlocal hydrodynamic Drude model [as described mathematically in (5)] has been extended to account for the classical kinetic effects of the charge carrier diffusion in the nonlocal response. This so-called generalized nonlocal optical response (GNOR) model expresses the relationship between $\mathbf{J}_H(\mathbf{r})$ and $\mathbf{E}(\mathbf{r})$ as follows:

$$\begin{aligned} [\beta^2 + D(\gamma + j\omega)]\nabla[\nabla \cdot \mathbf{J}_H(\mathbf{r})] + \omega(\omega - j\gamma)\mathbf{J}_H(\mathbf{r}) \\ = -j\omega\omega_p^2\varepsilon_0\mathbf{E}(\mathbf{r}), \quad \mathbf{r} \in V_H. \end{aligned} \quad (23)$$

Here, β , γ , and ω_p are the same as those in (5) and the additional parameter D is the charge carrier diffusion constant. Comparing (5) and (23), one can easily see that the only difference between the two equations is the additional term $D(\gamma + j\omega)$ in (23). Furthermore, both the nonlocal models use the same boundary condition given in (6). Therefore, the implementation of the GNOR model within the numerical scheme proposed here is rather trivial and can simply be done by replacing β^2 by $\beta^2 + D(\gamma + j\omega)$.

- 3) In [41] and [42], an analytical method that relies on the Mie series expansion of the fields has been used to study the nonlocal response of nanospheres in three different scenarios: electromagnetic scattering, electron energy-loss spectroscopy, and atomic spontaneous emission. Even though examples presented in Section III involve only electromagnetic scattering problems under plane-wave excitation, the proposed numerical scheme

is applicable to other problems with different types of excitation, including electron energy-loss and atomic spontaneous emission.

III. NUMERICAL RESULTS

In this Section, several numerical examples are presented to demonstrate the accuracy, the efficiency, and the applicability of the proposed solver. All the scatterers considered in these examples reside in free space with permittivity ε_0 and permeability μ_0 . For all the examples, the excitation is a plane wave with electric field

$$\mathbf{E}^{\text{inc}}(\mathbf{r}) = \hat{\mathbf{p}} E_0 e^{-j\mathbf{k}^{\text{inc}} \cdot \mathbf{r}}. \quad (24)$$

Here, the unit vector $\hat{\mathbf{p}}$ represents the direction of the polarization, E_0 is the electric field amplitude, and the unit vector $\hat{\mathbf{k}}^{\text{inc}}$ represents the direction of propagation. Unless otherwise stated, $\hat{\mathbf{p}} = \hat{\mathbf{x}}$, $E_0 = 1$ V/m, and $\hat{\mathbf{k}}^{\text{inc}} = \hat{\mathbf{z}}$ for all the examples considered here. All the TFQMR iterations (outer and inner iterations for the two-level iterative solver and the iterations for the single-level iterative solver) are terminated when the relative residual error (RRE) reaches a desired level, i.e., when the condition $\|\mathbf{b} - \mathbf{A}\mathbf{I}_n\|/\|\mathbf{b}\| \leq \chi_{\text{RRE}}$ is satisfied. Here, \mathbf{I}_n is the solution at iteration step n , \mathbf{A} is the matrix, \mathbf{b} is the right-hand side vector, and χ_{RRE} is the convergence threshold.

A. Metallic Sphere

In this example, electromagnetic scattering from a gold nanosphere [Fig. 3(a)] is analyzed using the proposed method. The radius of the sphere is 1 nm. The hydrodynamic equation parameters for gold are $\omega_p = 1.20 \times 10^{16}$ s⁻¹, $\gamma = 1.36 \times 10^{14}$ s⁻¹, $v_F = 1.39 \times 10^6$ m/s, and $\varepsilon_b(\mathbf{r}) = 1$ [36]. Note that for this problem, $V_D = V_H$ and $V_{\text{diel}} = \emptyset$.

Two sets of simulations are carried out. For the first set of simulations, frequency is set to $\omega = 0.5\omega_p$ and three levels of mesh are used. These meshes use $N_D = \{5494, 9216, 17546\}$ and $N_H = \{5030, 8612, 16694\}$ basis functions to discretize $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ induced inside the sphere, respectively. The single-level and two-level iterative schemes are used to solve the matrix system (12), which is preconditioned from left using a diagonal preconditioner, and the matrix system (20), respectively. For the iterations of the single-level scheme and the outer iterations of the two-level scheme, $\chi_{\text{RRE}} = 10^{-4}$. For the inner iterations of the two-level scheme, $\chi_{\text{RRE}} = 10^{-8}$. Note that the accuracy of the inner iterations has to be high to ensure that the outer iterations converge. This does not increase the computational cost significantly because the converge rate of the inner iterations is already very fast.

Fig. 3(b) shows plots of the radar cross section (RCS) computed on the xy -plane from the solutions obtained by the single-level and two-level iterative schemes for the mesh with $N_D = 17546$ and $N_H = 16694$ and the analytical Mie series with nonlocal response material model [43], [44]. The results agree very well. Table I shows comparison of the performance of the single-level and two-level iterative solvers. The two-level iterative solver is significantly faster due to fact that $N_{\text{it}}^{\text{out}}$ is much smaller than N_{it} and $N_{\text{it}}^{\text{in}}$ is small (see the computational complexity comparison in Section II-C). Note that the numbers for $N_{\text{it}}^{\text{in}}$ presented in Table I are the range of the inner iterations.

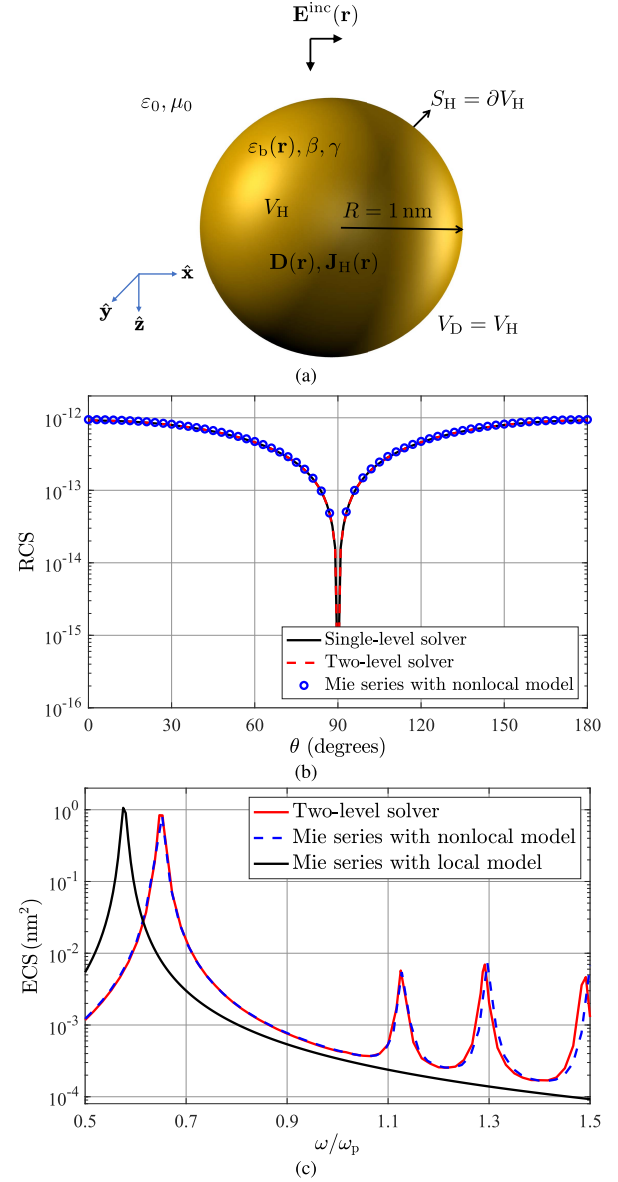


Fig. 3. (a) Description of the scattering problem involving a gold nanosphere. (b) RCS computed on the xy -plane at $\omega = 0.5\omega_p$ from the solutions obtained using the single-level and two-level iterative schemes and the Mie series with nonlocal response material. (c) ECS computed from the solutions obtained using the two-level iterative scheme and the Mie series with nonlocal and local response material models versus ω/ω_p .

TABLE I
PERFORMANCE OF THE SINGLE-LEVEL AND TWO-LEVEL ITERATIVE SOLVERS IN ANALYZING SCATTERING FROM A GOLD NANOSPHERE

Mesh levels		Single-level iterative solver		Two-level iterative solver		
N_D	N_H	Time (s)	N_{it}	Time (s)	$N_{\text{it}}^{\text{out}}$	$N_{\text{it}}^{\text{in}}$
5 494	5 030	29	84	10	29	30 – 35
9 216	8 612	105	108	32	26	35 – 40
17 546	16 694	530	126	106	24	45 – 50

For the second set of simulations, a total of 60 simulations are carried out using the two-level iterative solver at equally spaced points in the frequency range $\omega \in [0.5\omega_p, 1.5\omega_p]$. In these simulations, $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ induced inside the sphere

are discretized using $N_D = 143\,254$ and $N_H = 140\,022$ basis functions, respectively. For the outer and inner iterations of the two-level iterative scheme, $\chi_{\text{RRE}} = 10^{-4}$ and $\chi_{\text{RRE}} = 10^{-8}$, respectively.

Fig. 3(c) shows plots of the extinction cross section (ECS) computed from the solutions obtained using the two-level iterative scheme and the analytical Mie series with nonlocal and local response material models versus ω/ω_p [43], [44]. The figure clearly shows that the result obtained using the proposed method matches well with the result obtained using the Mie series with the nonlocal response material model. The figure also shows that the error in the result obtained by the proposed method increases with ω . This error can be reduced using a denser mesh that can capture the behavior of the fields with large $k_L(\mathbf{r})$ more accurately (see Section II-D and Fig. 2).

The first peak observed in all three ECS curves is caused by the transverse field resonance. Also, a “blue shift” phenomenon is shown in this figure, i.e., the transverse field resonance peak shifts toward higher frequencies when the nonlocal material response is taken into account [40]. Furthermore, three other peaks are identified at $\omega = 1.13\omega_p$, $\omega = 1.29\omega_p$, and $\omega = 1.50\omega_p$ in ECS computed by the proposed solver and the Mie series with the nonlocal response material model. These are caused by the longitudinal field resonance. It also can be concluded from Fig. 3(c) that the transverse field response is more dominant at $\omega < \omega_p$ while the longitudinal field response is more dominant at $\omega > \omega_p$.

B. Metallic Dimer

In this example, electromagnetic scattering from a nanodimer [Fig. 4(a)] is analyzed using the proposed solver. The radius of the spheres is 1 nm, and the shortest distance between them is 0.2 nm. The hydrodynamic equation parameters for the material making up the spheres are $\omega_p = 1.20 \times 10^{16} \text{ s}^{-1}$, $\gamma = 1.36 \times 10^{14} \text{ s}^{-1}$, $v_F = 1.39 \times 10^6 \text{ m/s}$, and $\varepsilon_b(\mathbf{r}) = 1$. Note that for this problem, $V_D = V_H$ and $V_{\text{diel}} = \emptyset$.

A total of 60 simulations are carried out using the two-level iterative scheme at equally spaced points in the frequency range $\omega \in [0.5\omega_p, 1.5\omega_p]$. Both the spheres use the same mesh of tetrahedrons and two levels of mesh are used. For simulations at $\omega < \omega_p$, $N_D = 104\,194$ and $N_H = 100\,706$, while for simulations at $\omega > \omega_p$, $N_D = 286\,958$ and $N_H = 280\,494$. For the outer and inner iterations of the two-level iterative scheme, $\chi_{\text{RRE}} = 10^{-4}$ and $\chi_{\text{RRE}} = 10^{-8}$, respectively.

Fig. 4(b) shows plots of the scattering cross section (SCS) computed from the solutions obtained using the two-level iterative scheme versus ω/ω_p [45]. The transverse field resonance peaks are observed at $\omega = 0.6\omega_p$ and $\omega = 0.75\omega_p$, while the longitudinal field resonance peaks are observed at $\omega = 1.13\omega_p$, $\omega = 1.29\omega_p$, and $\omega = 1.50\omega_p$. Furthermore, the figure shows that the nanodimer supports bonding and anti-bonding modes (generated by the transverse field resonances) at $\omega = 0.72\omega_p$ and $\omega = 0.75\omega_p$, respectively [15].

C. Composite Sphere

In this example, electromagnetic scattering from a silica-coated gold nanosphere [Fig. 5(a)] is analyzed using the proposed solver. The radius of the gold sphere is 1 nm, and

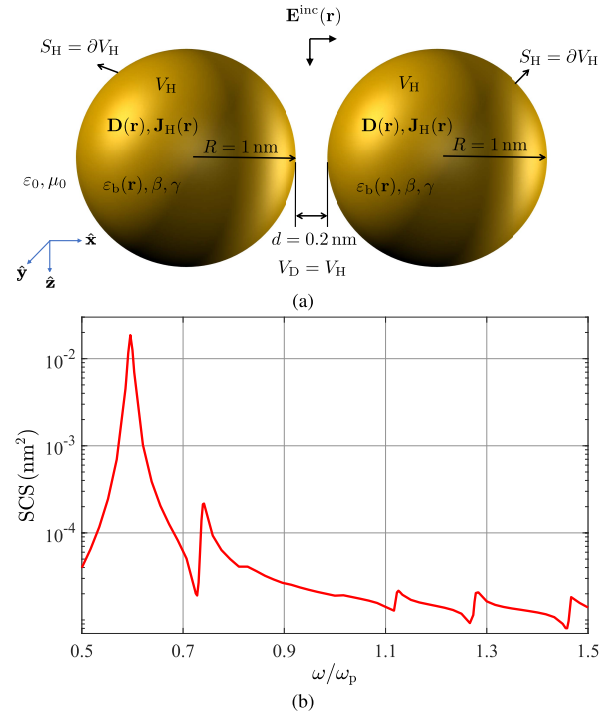


Fig. 4. (a) Description of the scattering problem involving a nanodimer. (b) SCS computed from the solutions obtained using the two-level iterative scheme versus ω/ω_p .

the thickness of the silica coating is 1 nm. The hydrodynamic equation parameters for gold are the same as those in Section III-A, and the relative permittivity of silica is $\varepsilon_b(\mathbf{r}) = 2.25$. Note that for this problem, $V_D = V_{\text{diel}} \cup V_H$.

A total of 60 simulations are carried out using the two-level iterative scheme at equally spaced points in the frequency range $\omega \in [0.4\omega_p, 1.4\omega_p]$. In these simulations, $\mathbf{D}(\mathbf{r})$ induced inside the coating and the sphere and $\mathbf{J}_H(\mathbf{r})$ induced inside the sphere are discretized using $N_D = 97\,642$ and $N_H = 80\,486$ basis functions, respectively. For the outer and inner iterations of the two-level iterative scheme, $\chi_{\text{RRE}} = 10^{-4}$ and $\chi_{\text{RRE}} = 10^{-8}$, respectively.

Fig. 5(b) shows plots of ECS computed from the solutions obtained by the two-level iterative scheme and the Mie series with nonlocal response material model for the sphere and local response material model for the coating versus ω/ω_p . The results agree well; however, as expected, the error in the result obtained by the proposed method increases with ω . This error can be reduced using a denser mesh that can capture the behavior of the fields with large $k_L(\mathbf{r})$ more accurately (see Section II-D and Fig. 2).

The transverse field resonance peak is observed at $\omega = 0.55\omega_p$ and the longitudinal field resonance peaks are observed at $\omega = 1.13\omega_p$ and $\omega = 1.31\omega_p$. Comparing Figs. 3(c) and 5(b), one can see that the transverse field resonance peak shifts toward lower frequencies due to the presence of silica coating.

D. Metallic Cylinder

In this example, electromagnetic scattering from a gold nanocylinder [Fig. 6(a)] is analyzed using the

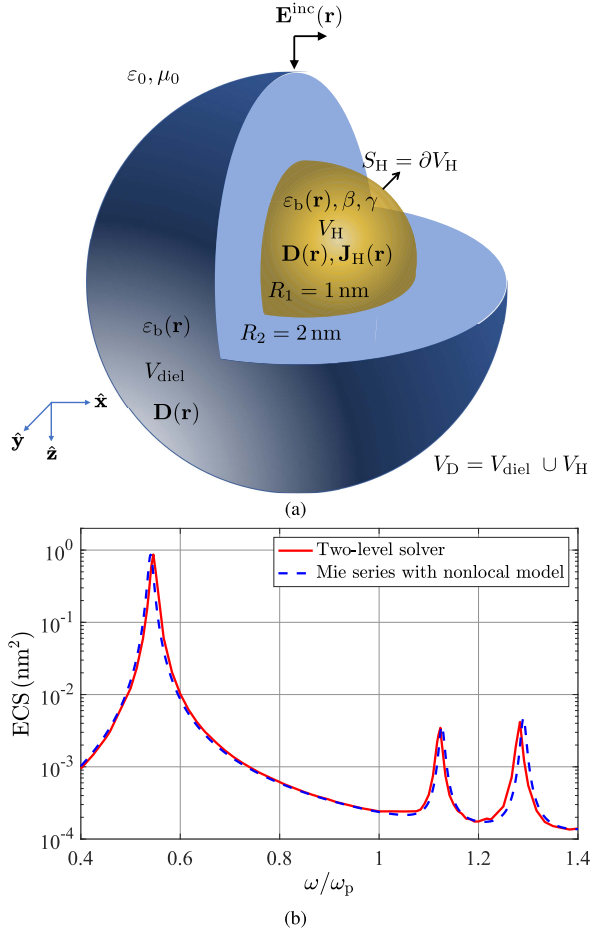


Fig. 5. (a) Description of the scattering problem involving a silica-coated gold nanosphere. (b) ECS computed from the solutions obtained using the two-level iterative scheme and the Mie series with nonlocal response material for the sphere and local response material for the coating versus ω/ω_p .

proposed method. Note that the ends of the cylinder are rounded here since sharp edges cannot be often fabricated at nanoscales. Four nanocylinders with length $H \in \{2.5 \text{ nm}, 3 \text{ nm}, 4 \text{ nm}, \text{ and } 5 \text{ nm}\}$ are considered. All the four cylinders have a radius of 1 nm. The hydrodynamic equation parameters for gold are the same as those in Section III-A. Note that for this problem, $V_D = V_H$ and $V_{\text{diel}} = \emptyset$.

A total of 60 simulations are carried out using the two-level iterative scheme at equally spaced points in the frequency range $\omega \in [0.5\omega_p, 1.25\omega_p]$. Four levels of mesh are used for the four nanocylinders and these meshes use $N_D = \{58\,312, 60\,948, 61\,010, 62\,186\}$ and $N_H = \{56\,384, 58\,900, 58\,962, 60\,006\}$ basis functions to discretize $\mathbf{D}(\mathbf{r})$ and $\mathbf{J}_H(\mathbf{r})$ induced inside the cylinder, respectively. For the outer and inner iterations of the two-level iterative scheme, $\chi_{\text{RRE}} = 10^{-4}$ and $\chi_{\text{RRE}} = 10^{-8}$, respectively.

Fig. 6(b) show compares of ECS computed from the solutions obtained using the two-level iterative scheme for all the four nanocylinders versus ω/ω_p . As seen from the figure, the transverse field resonance peak shifts from $\omega = 0.67\omega_p$ to $\omega = 0.69\omega_p$ when the length of the cylinder is increased from 2.5 to 5 nm. The longitudinal field resonance peaks are observed at $\omega = 1.1\omega_p$ and $\omega = 1.25\omega_p$. In addition, this figure shows an extra resonance peak that shifts from

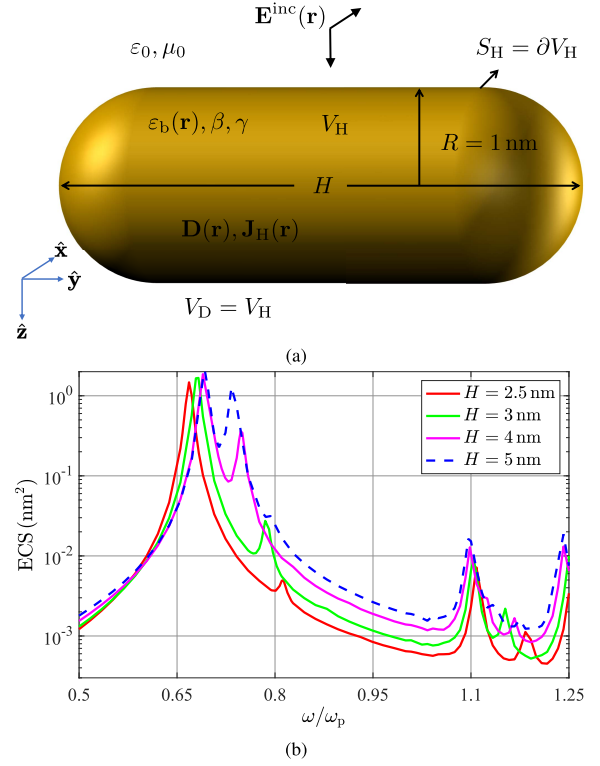


Fig. 6. (a) Description of the scattering problem involving a gold nanocylinder. (b) ECS computed from the solutions obtained using the two-level iterative scheme for all the four nanocylinders versus ω/ω_p .

$\omega = 0.81\omega_p$ to $\omega = 0.73\omega_p$ with increasing length. Note that this resonance (associated with the length of the cylinder along the \hat{y} -direction) is induced even though the incident electric field $\mathbf{E}^{\text{inc}}(\mathbf{r})$ is polarized in the \hat{x} -direction.

E. Metallic Cylinder on Top of a Dielectric Slab

For the last example, electromagnetic scattering from a gold nanocylinder located on top of a silica substrate [Fig. 7(a)] is analyzed using the proposed method. The length and the radius of the cylinder are 4 and 1 nm, respectively. The width, the length, and the height of the slab are 6, 6, and 1 nm, respectively. The shortest distance between the cylinder and the slab is 2 nm. The hydrodynamic equation parameters for gold are the same as those in Section III-A, and the relative electric permittivity of silica is $\varepsilon_b(\mathbf{r}) = 2.25$.

Three scattering scenarios are considered: 1) the scatterer is only the nanocylinder ($V_D = V_H$, $V_{\text{diel}} = \emptyset$, $N_D = 61\,010$, and $N_H = 58\,962$); 2) the scatterer consists of the nanocylinder and the substrate ($V_D = V_{\text{diel}} \cup V_H$, $N_D = 61\,294$, and $N_H = 58\,962$); and 3) the scatterer is only the substrate ($V_D = V_{\text{diel}}$, $V_H = \emptyset$, $N_D = 284$, and $N_H = 0$). The simulations of these three scenarios are carried out using the two-level iterative scheme [reduces to a “traditional” volume integral equation solver [46], [47] with single-level iterations for scenario (iii)] at 60 equally spaced points in the frequency range $\omega \in [0.5\omega_p, 1.25\omega_p]$. Note that for scenarios (ii) and (iii), only 284 basis functions are used to discretize $\mathbf{D}(\mathbf{r})$ induced inside the slab (see the discussion in Section II-D). For the outer and inner iterations of the two-level iterative scheme, $\chi_{\text{RRE}} = 10^{-4}$ and $\chi_{\text{RRE}} = 10^{-8}$, respectively.

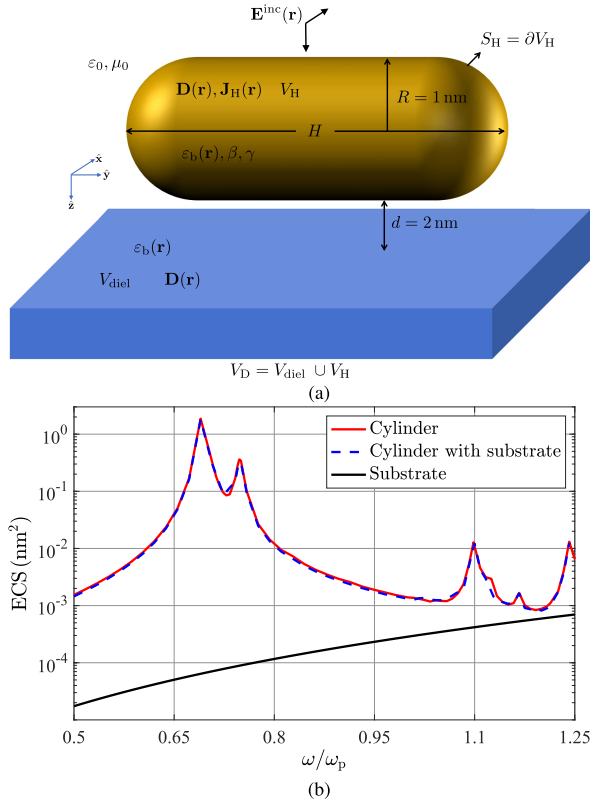


Fig. 7. (a) Description of the scattering problem involving a gold nanocylinder on top of a silica cylinder. (b) ECS computed from the solutions obtained in all three scenarios (the scatterer consists of only the cylinder, the cylinder and the substrate, and only the substrate) versus ω/ω_p .

Fig. 7(b) shows plots of ECS computed in the three scenarios described above versus ω/ω_p . As expected, ECS of the silica slab [scenario (iii)] does not involve any resonance peaks since silica does not have any plasmonic properties. Second, the slab is located far away from the gold nanocylinder, so the coupling between them is not expected to be strong, and ECS in scenario (i) and ECS in scenario (ii) are close to each other especially at the lower end of the frequency range. The difference increases at the higher end, which might be explained by the fact that ECS of the silica slab is larger at higher frequencies [scenario (iii)] and therefore contributes more to the total ECS in scenario (ii).

IV. CONCLUSION

Electromagnetic scattering from nanostructures consisting of the metallic and dielectric parts is analyzed by solving a coupled system of the volume integral and hydrodynamic equations. The hydrodynamic equation, which is enforced only in the metallic part, relates the free electron polarization current to the electric flux. This equation effectively updates the constitutive relationship and permits modeling of the nonlocality. The volume integral equation, which is enforced in both the metallic and dielectric parts, relates the electric flux to the scattered electric field. Unknown electric flux and free electron polarization current are expanded using a combination of full and half SWG basis functions. The boundary condition associated with the free electron polarization current on the

metal–dielectric interface is enforced by excluding the half SWG basis functions, which are located on this interface, from the expansion of the free electron polarization current. Inserting these expansions into the coupled system of the volume integral and hydrodynamic equations and using Galerkin testing yield a matrix system.

An efficient two-level iterative solver is developed to solve this matrix system. This approach inverts the discretized hydrodynamic equation (bottom rows of the matrix system) for the coefficients of the free electron polarization current and substitutes the result in the discretized volume integral equation (top rows of the matrix system). Outer iterations solve this reduced matrix system, while the inner iterations invert the discretized hydrodynamic equation at every iteration of the outer iterations.

Numerical experiments, which involve the computation of RCS, ECS, and SCS for metallic and composite nanostructures, are carried out to demonstrate the accuracy, the efficiency, and the applicability of the proposed method.

Future research directions include incorporation of different nonlocal hydrodynamic equations, implementation of boundary conditions on metal–metal interfaces, acceleration of the matrix solution using matrix compression schemes, and application of the proposed solver to different problems with different types of excitations.

APPENDIX

ENTRIES OF THE MATRIX AND THE RIGHT-HAND SIDE VECTOR IN (12)

While computing the entries of \mathbf{Z}_{DD} , \mathbf{Z}_{DH} , \mathbf{Z}_{HD} , and \mathbf{Z}_{HH} , it is assumed that $\varepsilon_b(\mathbf{r})$ and $\kappa(\mathbf{r})$ are constant in a given tetrahedron, and the values of these constants are obtained by sampling $\varepsilon_b(\mathbf{r})$ and $\kappa(\mathbf{r})$ at the center of that tetrahedron. Therefore, one can define local functions as follows:

$$\varepsilon_{b,n}(\mathbf{r}) = \begin{cases} \varepsilon_{b,n}^+ = \varepsilon_b(\mathbf{r}_c^+), & \mathbf{r} \in V_n^+ \\ \varepsilon_{b,n}^- = \varepsilon_b(\mathbf{r}_c^-), & \mathbf{r} \in V_n^- \end{cases}$$

$$\kappa_n(\mathbf{r}) = \begin{cases} \kappa_n^+ = \kappa(\mathbf{r}_c^+), & \mathbf{r} \in V_n^+ \\ \kappa_n^- = \kappa(\mathbf{r}_c^-), & \mathbf{r} \in V_n^- \end{cases}$$

where \mathbf{r}_c^\pm are the centers of V_n^\pm .

A. Entries of \mathbf{Z}_{DD}

If both $\mathbf{f}_m^D(\mathbf{r})$ and $\mathbf{f}_n^D(\mathbf{r})$ are full SWG functions, then

$$\begin{aligned} \{\mathbf{Z}_{DD}\}_{mn} &= \frac{1}{\varepsilon_0} \int_{V_m} \frac{\mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv \\ &\quad - \omega^2 \mu_0 \int_{V_m} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n} \kappa_n(\mathbf{r}') \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' dv \\ &\quad + \frac{1}{\varepsilon_0} \int_{V_m} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n} \kappa_n(\mathbf{r}') \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \left. - (\kappa_n^+ - \kappa_n^-) \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} dv. \end{aligned}$$

If $\mathbf{f}_m^D(\mathbf{r})$ is a half SWG function and $\mathbf{f}_n^D(\mathbf{r})$ is a full SWG function, then

$$\begin{aligned} \{\mathbf{Z}_{DD}\}_{mn} &= \frac{1}{\varepsilon_0} \int_{V_m^+} \frac{\mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv \\ &\quad - \omega^2 \mu_0 \int_{V_m^+} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n} \kappa_n(\mathbf{r}') \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' dv \\ &\quad + \frac{1}{\varepsilon_0} \int_{V_m^+} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n} \kappa_n(\mathbf{r}') \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - (\kappa_n^+ - \kappa_n^-) \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} dv \\ &\quad - \frac{1}{\varepsilon_0} \int_{S_m} \hat{\mathbf{n}}_m(\mathbf{r}) \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n} \kappa_n(\mathbf{r}') \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - (\kappa_n^+ - \kappa_n^-) \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} ds. \end{aligned}$$

Here, $\hat{\mathbf{n}}_m(\mathbf{r})$ is the unit normal vector on S_m pointing from V_n^- to V_n^+ and $\hat{\mathbf{n}}_m(\mathbf{r}) \cdot \mathbf{f}_m^D(\mathbf{r}) = 1$. If $\mathbf{f}_m^D(\mathbf{r})$ is a full SWG function and $\mathbf{f}_n^D(\mathbf{r})$ is a half SWG function, then

$$\begin{aligned} \{\mathbf{Z}_{DD}\}_{mn} &= \frac{1}{\varepsilon_0 \varepsilon_{b,n}^+} \int_{V_m} \mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r}) dv \\ &\quad - \omega^2 \mu_0 \kappa_n^+ \int_{V_m} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n^+} \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' dv \\ &\quad + \frac{\kappa_n^+}{\varepsilon_0} \int_{V_m} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n^+} \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} dv. \end{aligned}$$

If both $\mathbf{f}_m^D(\mathbf{r})$ and $\mathbf{f}_n^D(\mathbf{r})$ are half SWG functions, then

$$\begin{aligned} \{\mathbf{Z}_{DD}\}_{mn} &= \frac{1}{\varepsilon_0 \varepsilon_{b,n}^+} \int_{V_m^+} \mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r}) dv \\ &\quad - \omega^2 \mu_0 \kappa_n^+ \int_{V_m^+} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n^+} \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' dv \\ &\quad + \frac{\kappa_n^+}{\varepsilon_0} \int_{V_m^+} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n^+} \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} dv \\ &\quad - \frac{\kappa_n^+}{\varepsilon_0} \int_{S_m} \hat{\mathbf{n}}_m(\mathbf{r}) \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n^+} \nabla' \cdot \mathbf{f}_n^D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} ds. \end{aligned}$$

B. Entries of \mathbf{Z}_{DH}

$\mathbf{f}_n^H(\mathbf{r})$ is always a full SWG function. If $\mathbf{f}_m^D(\mathbf{r})$ is a full SWG function, then

$$\begin{aligned} \{\mathbf{Z}_{DH}\}_{mn} &= -\frac{1}{j\omega\varepsilon_0} \int_{V_m} \frac{\mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^H(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv \\ &\quad + j\omega\mu_0 \int_{V_m} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n} \frac{\mathbf{f}_n^H(\mathbf{r}')}{\varepsilon_{b,n}(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dv' dv \end{aligned}$$

$$\begin{aligned} &+ \frac{1}{j\omega\varepsilon_0} \int_{V_m} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n} \frac{\nabla' \cdot \mathbf{f}_n^H(\mathbf{r}')}{\varepsilon_{b,n}(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \left. - \left[\frac{1}{\varepsilon_{b,n}^+} - \frac{1}{\varepsilon_{b,n}^-} \right] \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} \\ &\quad \times dv. \end{aligned}$$

If $\mathbf{f}_m^D(\mathbf{r})$ is a half SWG function, then

$$\begin{aligned} \{\mathbf{Z}_{DH}\}_{mn} &= -\frac{1}{j\omega\varepsilon_0} \int_{V_m^+} \frac{\mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{f}_n^H(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv \\ &\quad + j\omega\mu_0 \int_{V_m^+} \mathbf{f}_m^D(\mathbf{r}) \cdot \int_{V_n} \frac{\mathbf{f}_n^H(\mathbf{r}')}{\varepsilon_{b,n}(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dv' dv \\ &\quad + \frac{1}{j\omega\varepsilon_0} \int_{V_m^+} \nabla \cdot \mathbf{f}_m^D(\mathbf{r}) \left\{ \int_{V_n} \frac{\nabla' \cdot \mathbf{f}_n^H(\mathbf{r}')}{\varepsilon_{b,n}(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - \left[\frac{1}{\varepsilon_{b,n}^+} - \frac{1}{\varepsilon_{b,n}^-} \right] \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} dv \\ &\quad - \frac{1}{j\omega\varepsilon_0} \int_{S_m} \hat{\mathbf{n}}_m(\mathbf{r}) \cdot \mathbf{f}_m^D(\mathbf{r}) \\ &\quad \times \left\{ \int_{V_n} \frac{\nabla' \cdot \mathbf{f}_n^H(\mathbf{r}')}{\varepsilon_{b,n}(\mathbf{r}')} G(\mathbf{r}, \mathbf{r}') dv' \right. \\ &\quad \quad \left. - \left[\frac{1}{\varepsilon_{b,n}^+} - \frac{1}{\varepsilon_{b,n}^-} \right] \int_{S_n} G(\mathbf{r}, \mathbf{r}') ds' \right\} ds. \end{aligned}$$

C. Entries of \mathbf{Z}_{HD}

$\mathbf{f}_n^H(\mathbf{r})$ is always a full SWG function. If $\mathbf{f}_n^D(\mathbf{r})$ is a full SWG function, then

$$\{\mathbf{Z}_{HD}\}_{mn} = j\omega\omega_p^2 \int_{V_m} \frac{\mathbf{f}_m^H(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv.$$

If $\mathbf{f}_n^D(\mathbf{r})$ is a half SWG function, then

$$\{\mathbf{Z}_{HD}\}_{mn} = \frac{j\omega\omega_p^2}{\varepsilon_{b,n}^+} \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathbf{f}_n^D(\mathbf{r}) dv.$$

D. Entries of \mathbf{Z}_{HH}

$\mathbf{f}_m^H(\mathbf{r})$ and $\mathbf{f}_n^H(\mathbf{r})$ are always full SWG functions

$$\begin{aligned} \{\mathbf{Z}_{HH}\}_{mn} &= -\beta^2 \int_{V_m} [\nabla \cdot \mathbf{f}_m^H(\mathbf{r})][\nabla \cdot \mathbf{f}_n^H(\mathbf{r})] dv \\ &\quad + \omega(\omega - j\gamma) \int_{V_m} \mathbf{f}_m^H(\mathbf{r}) \cdot \mathbf{f}_n^H(\mathbf{r}) dv \\ &\quad - \omega_p^2 \int_{V_m} \frac{\mathbf{f}_m^H(\mathbf{r}) \cdot \mathbf{f}_n^H(\mathbf{r})}{\varepsilon_{b,n}(\mathbf{r})} dv. \end{aligned}$$

E. Entries of \mathbf{V}^{inc}

If \mathbf{f}_m^D is a full SWG function, then

$$\{\mathbf{V}^{\text{inc}}\}_m = \int_{V_m} \mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{E}^{\text{inc}}(\mathbf{r}) dv.$$

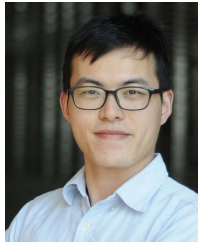
If \mathbf{f}_m^D is a half SWG function, then

$$\{\mathbf{V}^{\text{inc}}\}_m = \int_{V_m^+} \mathbf{f}_m^D(\mathbf{r}) \cdot \mathbf{E}^{\text{inc}}(\mathbf{r}) dv.$$

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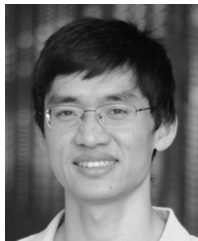
Doolos Aibek Uulu (Student Member, IEEE) received the B.S. degree in physics from Middle East Technical University (METU), Ankara, Turkey, in 2015, and the M.S. degree in material science and nanotechnology from Bilkent University, Ankara, in 2017. He is currently pursuing the Ph.D. degree in electrical and computer engineering program from the King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia. During the Ph.D. degree, his research focuses on computational electromagnetics to model plasmonic structures by combining volume integral equation and hydrodynamic equation.



Rui Chen (Member, IEEE) received the B.Eng. degree in communication engineering and the M.Eng. degree in electromagnetic field and microwave technology from the Nanjing University of Science and Technology, Nanjing, China, in 2010 and 2015, respectively, and the Ph.D. degree in Electrical and Computer Engineering from the King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, in 2021.

From June 2021 to April 2022, he was a Post-Doctoral Fellow with the Computational Electromagnetics Group, KAUST. Since May 2022, he has been a Post-Doctoral Fellow with the Computational Electromagnetics Research Laboratory, Politecnico di Turin, Turin, Italy. His research interests include various aspects of theoretical and applied computational electromagnetics with emphasis on well-conditioned frequency and time-domain integral equation formulations and their higher order discretization, and accurate, stable, and efficient marching-on-in-time schemes for time-domain integral equation solvers.

Dr. Chen received two Honorable Mention Awards at the Student Paper Competition of the IEEE Antennas and Propagation Society International Symposiums, in 2018 and 2020, respectively. He was one of the finalists at the Student Paper Competition of the 2019 Applied Computational Electromagnetics Society Conference. He was one of the recipients of the Gauss Centre for Supercomputing Award presented at the 2020 International Supercomputing Conference High Performance. He was the recipient of the 2021 International Union of Radio Science (URSI) Young Scientist Award presented at the XXXIVth URSI General Assembly.



Liang Chen (Senior Member, IEEE) received the B.S. degree in applied physics from Southeast University, Nanjing, China, in 2007, and the M.S. and Ph.D. degrees in microelectronic and solid-state electronics from the Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai, China, in 2009 and 2012, respectively.

From 2012 to 2013, he was a High-Performance Computing (HPC) Engineer with the HPC Solution Center of Dawning Information Industry Company Ltd. From 2013 to 2017, he was the Technical Solution Department Manager with DongJun Technology Company Ltd., and a Principal Developer with the Electromagnetic Simulation Software East Wave, Shanghai. In 2017, he joined the King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, as a Post-Doctoral Research Fellow. Since 2020, he has been a Research Scientist at KAUST. His research interests include computational physics (electromagnetics, semiconductor devices, quantum transport, and multiphysics simulation), computer-aided engineering software, high-performance computing, and various topics in photonics and condensed matter physics.



Ping Li (Senior Member, IEEE) received the B.S. degree in physical electronics engineering and the master's degree from the University of Electronic Science and Technology of China (UESTC), Chengdu, China, in 2008 and 2010, respectively, and the Ph.D. degree in electrical and electronic engineering from The University of Hong Kong (HKU), Hong Kong, in 2014.

From October 2014 to December 2015, he was a Post-Doctoral Fellow at the Computational Electromagnetics Laboratory, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia. From December 2015 to December 2016, he was a Post-Doctoral Fellow at the On-Chip Electromagnetics Laboratory, Purdue University, West Lafayette, IN, USA.

From January 2017 to August 2018, he joined with the Department of Electrical and Electronic Engineering, HKU as a Research Assistant Professor. From September 2018 to August 2019, he was a Research Scientist with the KAUST as well as a Honorary Assistant Professor at the HKU. Since August 2019, he has been with Shanghai Jiao Tong University, Shanghai, China, as an Associate Professor.

Dr. Li was a recipient of the 2018 Joint IEEE EMC and APEMC Outstanding Young Scientist Award, the 2018 ACES-China Young Scientist Award, the 40th PIERS Young Scientist Award in Japan, the Okawa Research Foundation Grant of Japan, the 2018 Best Annual Paper Prize on *Chinese Journal of Radio Science*, and the Second Prize Award for Natural Sciences of Chinese Institute of Electronics, in 2019. Besides, his paper was selected as the Finalist paper in 29th International Review of Progress in Applied Computational Electromagnetics and the 2014 International Symposium on Electromagnetic Compatibility, and he won the Best Student Paper Award in 12th International Workshop on Finite Elements for Microwave Engineering.



Hakan Bagci (Senior Member, IEEE) received the B.S. degree in electrical and electronics engineering from Bilkent University, Ankara, Turkey, in 2001, and the M.S. and Ph.D. degrees in electrical and computer engineering from the University of Illinois at Urbana-Champaign (UIUC), Urbana, IL, USA, in 2003 and 2007, respectively.

From June 1999 to July 2001, he worked as an Undergraduate Researcher with the Computational Electromagnetics Group, Bilkent University. From August 2001 to December 2006, he was a Research Assistant with the Center for Computational Electromagnetics and Electromagnetics Laboratory, UIUC. From January 2007 to August 2009, he was a Research Fellow with the Radiation Laboratory, University of Michigan, Ann Arbor, MI, USA. Since August 2009, he has been with the King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia, where he is currently an Associate Professor of electrical and computer engineering. He has authored or coauthored around 120 journal articles and 250 contributions in conference proceedings. His research interests include various aspects of theoretical and applied computational electromagnetics with emphasis on well-conditioned frequency and time-domain integral equation formulations and their discretization, hybrid time-domain integral and differential equation solvers, accurate, stable, and efficient marching schemes for time-domain solvers, stochastic characterization of electromagnetic field and wave interactions on complex geometries, and solution of 2-D and 3-D electromagnetic inverse scattering problem using signal processing techniques.

Dr. Bagci is a Senior Member of the URSI Commission B and a fellow of the Applied Computational Electromagnetics Society (ACES). He was a recipient of the 2008 International Union of Radio Scientists (URSI) Young Scientist Award presented at the XXIXth URSI General Assembly and the 2004–2005 Interdisciplinary Graduate Fellowship from the Computational Science and Engineering Department, UIUC. His paper titled “Fast and Rigorous Analysis of EMC/EMI Phenomena on Electrically Large and Complex Structures Loaded With Coaxial Cables” was one of the three finalists (with honorable mention) for the 2008 Richard B. Schulz Best Transactions Paper Award given by the IEEE Electromagnetic Compatibility Society. He has authored (as student) or coauthored (as student and advisor) 18 finalist/honorable mention papers in the student paper competitions at the 2005, 2008, 2010, 2014–2018, and 2020 IEEE Antennas and Propagation Society International Symposiums and 2013–2019 Applied Computational Electromagnetics Society Conferences. In 2020, he was one of the recipients of the Gauss Center for Supercomputing (GSC) Award for the paper titled “Solving Acoustic Boundary Integral Equations Using High Performance Tile Low-Rank LU Factorization” and presented at the International Supercomputing Conference (ISC) High Performance. In 2021, he received the KAUST Distinguished Teaching Award. He has organized and chaired many sessions at IEEE Antennas and Propagation Society International Symposiums and Applied Computational Electromagnetics Society Conferences. More recently, he served as a Vice Chair (responsible for computational electromagnetics track) of the technical program committee for the IEEE Antennas and Propagation Society International Symposium that was held in Atlanta, GA, USA, in July 2019. He is currently an Associate Editor of IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, IEEE JOURNAL ON MULTISCALE AND MULTIPHYSICS COMPUTATIONAL TECHNIQUES, and *IEEE Antennas and Propagation Magazine*.