Windowed Green Function MoM for Second-Kind Surface Integral Equation Formulations of Layered Media Electromagnetic Scattering Problems

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Abstract—This article presents a second-kind surface integral equation (SIE) method for the numerical solution of frequency-domain electromagnetic (EM) scattering problems by locally perturbed layered media in three spatial dimensions. Unlike standard approaches, the proposed methodology does not involve the use of layer Green functions (LGFs). It instead leverages an indirect Müller formulation in terms of free-space Green functions that entails integration over the entire unbounded penetrable boundary. The integral equation domain is effectively reduced to a small-area surface by means of the windowed Green function (WGF) method, which exhibits high-order convergence as the size of the truncated surface increases. The resulting (second-kind) windowed integral equation is then numerically solved by means of the standard Galerkin method of moments (MoM) using the Rao–Wilton–Glisson (RWG) basis functions. The methodology is validated by comparison with the Mie series and Sommerfeld integral exact solutions as well as against the LGF-based MoM. Challenging examples including realistic artificial/transparent interfaces need to be introduced to properly represent the fields surrounding the perturbations. In many application areas it is crucial to determine the scattering from localized perturbations (e.g., surface roughness, small-size inclusions, meta-atoms) and/or the field produced by localized sources (e.g., antenna feeds) embedded within physically large structures that away from a certain region of interest can be effectively assumed as planar and infinite (e.g., the surface of the Earth, silicon substrates). This is often the case in numerous problems in radio communications, remote subsurface sensing, microwave circuits, nano-optical metamaterials, photonics, and plasmonics.

Index Terms—Dielectric cavities, layer Green function (LGF), layered media, metasurfaces, method of moments (MoM), solar cells, Sommerfeld integrals.

I. INTRODUCTION

Problems of electromagnetic (EM) scattering and radiation in the presence of planar layered media have played an important role in the development of EMs since the beginning of the 20th century, when the seminal works of Zenneck and Sommerfeld on the propagation of radio waves over the surface of the Earth appeared [1]. Their relevance lies in that in
the use of Sommerfeld integrals or other problem-specific Green functions. This is here achieved by first deriving an indirect Müller SIE [31], [32] given in terms of free-space Green functions and featuring only weakly singular kernels, which is posed on the entire unbounded penetrable interface (see Sections III and IV). The unbounded SIE domain is then effectively truncated to a bounded surface containing localized perturbations by introducing (in the surface integrals) a smooth windowing function that effectively acts like a reflectionless absorber for the surface currents leaving the windowed region (see Section V). As in the case of the Helmholtz SIEs [26], the field errors introduced by the windowing approximation decay faster than any negative power of the diameter of the truncated region. A straightforward (Galerkin) MoM discretization using Rao–Wilton–Glisson (RWG) functions is used to discretize the resulting windowed SIE (see Section VI), although any other Maxwell SIE method could be used. A limitation of the proposed approach is that the transmission conditions at unbounded penetrable interfaces need to be enforced via second-kind SIEs such as Müller’s. First-kind SIEs, such as the more popular Poggio–Müller–Chang–Harrington–Wu–Tsai (PMCHWT) [33], [34], [35], could be considered provided they are converted into equivalent second-kind SIEs by means of Calderón preconditioners [36].

Compared with the LGF-SIE formulations, the WGF formulation involves additional unknown surface currents on the planar portions of the unbounded dielectric interfaces that eventually lead to larger linear systems. In many cases, this additional cost is compensated by the fact that the associated matrix coefficients involve evaluations of the inexpensive free-space Green functions and that the resulting linear system can be efficiently solved iteratively by means of GMRES (see Section VII-C). For problems involving multiple dielectric layers and/or small-size PEC inclusions, however, LGF formulations that leverage the discrete complex images method (DCIM) [37], [38], [39] for the evaluation of the LGF may well outperform the WGF methodology.

The proposed approach amounts to a flexible and easy-to-implement MoM for layered media EM problems, in the sense that only minor modifications to the existing EM SIE solvers are needed to deliver the WGF capabilities. The method is thoroughly validated (see Section VII) against the exact Mie series scattering solution for a hemispherical bump on a penetrable locally perturbed half-space \( \Omega_2 \), with boundary \( \Gamma = \partial \Omega_2 \), as depicted in Fig. 1. Letting \( \Omega_1 = \mathbb{R}^3 \setminus \overline{\Omega_2} \), we express the total EM field as

\[
\begin{align*}
(E^{\text{tot}}, H^{\text{tot}}) &= (E^{\text{inc}}, H^{\text{inc}}) + (E_j, H_j) \quad \text{in } \Omega_j
\end{align*}
\]

for \( j = 1, 2 \). The known auxiliary source field \((E^{\text{inc}}, H^{\text{inc}})\) which is given in terms of the incident field \((E^{\text{inc}}, H^{\text{inc}})\) under consideration is constructed so that the fields \((E_j, H_j)\), \( j = 1, 2 \), satisfy the homogeneous Maxwell equations

\[
\nabla \times E_j - i \omega \mu_j H_j = 0 \quad \text{and } \nabla \times H_j + i \omega \varepsilon_j E_j = 0 \quad \text{in } \Omega_j
\]

for \( j = 1, 2 \), where \( \omega > 0 \) is the angular frequency, and \( \varepsilon_j \) and \( \mu_j \) are, respectively, the permittivity and the permeability within the subdomain \( \Omega_j \). (We have assumed here that the time dependence of the EM fields is given by \( e^{-i \omega t} \).) For plane wave incidences, for instance, \((E^{\text{inc}}, H^{\text{inc}})\) is taken as the exact total field solution of the problem of scattering of the plane wave by the flat lower half-space with planar boundary \( \Sigma = \{(x, y, 0) \in \mathbb{R}^3 \} \) and constants \( \varepsilon_2 \) and \( \mu_2 \) (see Fig. 1).

The rationale for introducing \((E^{\text{inc}}, H^{\text{inc}})\) lies in ensuring that \((E_j, H_j), j = 1, 2 \), are outgoing wavefields propagating away from localized perturbations or, more precisely, that they satisfy the Silver–Müller radiation condition

\[
|E_j| \leq \frac{\sqrt{\mu_j}}{|r|} \frac{\sqrt{e_j}}{r} \quad \text{uniformly in all the directions } r/|r|.
\]

The explicit expressions of the source fields used throughout the article are provided in Section III below.

The transmission conditions at the material interfaces, meaning that the tangential components of \((E^{\text{tot}}, H^{\text{tot}})\) are continuous across \( \Gamma \), lead to the jump conditions

\[
\begin{align*}
\hat{n} \times \{E_2|_\Gamma - E_1|_\Gamma\} &= M^{\text{inc}} \quad (4a) \\
\hat{n} \times \{H_2|_\Gamma - H_1|_\Gamma\} &= J^{\text{inc}} \quad (4b)
\end{align*}
\]

on \( \Gamma \), with

\[
\begin{align*}
M^{\text{inc}} := \hat{n} \times \{E^{\text{inc}}|_\Gamma - E^{\text{inc}}|_{\Gamma^-}\} \quad (5a) \\
J^{\text{inc}} := \hat{n} \times \{H^{\text{inc}}|_\Gamma - H^{\text{inc}}|_{\Gamma^-}\} \quad (5b)
\end{align*}
\]

where we have adopted the notation \( F(r)|_{\pm} = \lim_{\beta \to 0^+} F(r \pm \delta n(r)) \) for \( r \in \Gamma \). As usual, the unit normal vector at \( r \in \Gamma \) is denoted as \( \hat{n}(r) \) and is assumed directed from \( \Omega_2 \) to \( \Omega_1 \).

II. LAYERED MEDIA SCATTERING

We consider here the problem of time-harmonic EM scattering of an incident field \((E^{\text{inc}}, H^{\text{inc}})\) by a penetrable locally
III. INCIDENT AND SOURCE FIELDS

Two types of incident fields (\(E^{inc}, H^{inc}\)) and corresponding auxiliary source fields (\(E^{src}, H^{src}\)) are considered in this article, namely, planewaves and electric dipoles.

Upon impinging on the planar surface \(\Sigma\) at the interface between the half spaces \(D_1 = \{z > 0\}\) and \(D_2 = \{z < 0\}\) with wavenumbers \(k_1\) and \(k_2\) \((k_j = \omega \mu_j / c, j = 1, 2)\), respectively, the incident plane wave

\[
E^{inc}(r) = (p \times k)e^{ik \cdot r} \quad \text{and} \quad H^{inc}(r) = \frac{1}{i\omega \mu_j} k \times E^{inc}(r) \tag{6}
\]

with \(p = (p_x, p_y, p_z)\) and \(k = (0, k_{1z}, -k_{2z})\) where \(k_{1z} \geq 0\) and \(|k| = (k_{1z}^2 + k_{2z}^2)^{1/2} = k_1\), giving rise to a reflected field (\(E^{ref}, H^{ref}\)) in \(D_1\) and a transmitted field (\(E^{tr}, H^{tr}\)) in \(D_2\). The resulting \(x\)-independent total field, given by (\(E^{inc} + E^{ref}, \ H^{inc} + H^{ref}\)) in \(D_1\) and (\(E^{tr}, H^{tr}\)) in \(D_2\), is completely determined by the transverse component of the fields [43]

\[
\begin{align*}
E_{inc}^{x}(r) &= \begin{cases} E_{0}, & H_{0} \end{cases} \exp(ik_{1y}y - ik_{1z}z) \\
H_{inc}^{x}(r) &= \begin{cases} E_{0}, & H_{0} \end{cases} \exp(-ik_{1y}y + ik_{1z}z) \\
E_{ref}^{x}(r) &= \begin{cases} E_{0}R^{TE}, & H_{0}R^{TM} \end{cases} \exp(ik_{1y}y + ik_{1z}z) \\
H_{ref}^{x}(r) &= \begin{cases} E_{0}R^{TE}, & H_{0}R^{TM} \end{cases} \exp(-ik_{1y}y - ik_{1z}z)
\end{align*}
\]

depending on the reflection coefficients

\[
R^{TE} = \frac{\mu_2 k_{1z} - \mu_1 k_{2z}}{\mu_2 k_{1z} + \mu_1 k_{2z}}, \quad R^{TM} = \frac{\epsilon_2 k_{1z} - \epsilon_1 k_{2z}}{\epsilon_2 k_{1z} + \epsilon_1 k_{2z}}
\]

the transmission coefficients

\[
T^{TE} = \frac{2\mu_2 k_{12}}{\mu_2 k_{1z} + \mu_1 k_{2z}}, \quad T^{TM} = \frac{2\epsilon_2 k_{12}}{\epsilon_2 k_{1z} + \epsilon_1 k_{2z}}
\]

the amplitudes

\[
E_0 = -p_x k_{1y} - p_y k_{1z}, \quad H_0 = \frac{k_1^2}{i\omega \mu_1} p_x
\]

and the propagation constants \(k_{2y} = k_{1y}\) and \(k_{2z} = (k_{1z}^2 - k_{2z}^2)^{1/2}\) with the complex square root defined so that \(\text{Im} k_{2z} \geq 0\). The EM field can be retrieved from the transverse components via

\[
E = E_x \hat{x} + \frac{1}{i\omega \varepsilon_x} \frac{\partial H_x}{\partial z} \hat{y} + \frac{1}{i\omega \mu_x} \frac{\partial E_x}{\partial z} \hat{z},
\]

\[
H = H_x \hat{x} + \frac{1}{i\omega \mu_x} \frac{\partial E_x}{\partial z} \hat{y} + \frac{1}{i\omega \varepsilon_x} \frac{\partial H_x}{\partial z} \hat{z}.
\]

With these expressions at hand, we define the auxiliary planarwave source field as

\[
(E^{src}, H^{src}) = \begin{cases} (E^{inc}, H^{inc}) + (E^{ref}, H^{ref}), & \text{in } \Omega_1 \\
(E^{tr}, H^{tr}), & \text{in } \Omega_2. \end{cases} \tag{7}
\]

Since by construction the source field (7) satisfies the exact transmission conditions at \(\Sigma\), it holds that the current sources \(M^{src}\) and \(J^{src}\) defined in (5) are supported on the (bounded) local perturbation \(\Gamma'\). \(\Sigma\).

In the special case when \(\Omega_2\) is occupied by a PEC, in which the boundary condition \(\hat{n} \times E^{tot} = 0\) holds on the interface \(\Gamma\), we have that \((E^{src}, H^{src})\) takes the form (7) with \((E^{tr}, H^{tr}) = (0, 0)\) and \((E^{ref}, H^{ref})\) given in terms of the reflection coefficients \(R^{TE} = -R^{TM} = -1\).

Finally, we take

\[
H^{inc} = \frac{1}{i\omega \mu_j} \nabla \times \{G_j(\cdot, r_0) p\}, \quad E^{inc} = \frac{-1}{i\omega \varepsilon_j} \nabla \times H^{inc} \tag{8}
\]

with

\[
G_j (r, r') := \frac{e^{ik_j |r-r'|}}{4\pi |r-r'|} \tag{9}
\]

being the (Helmholtz) free-space Green function, as the incident field produced by an electric dipole at \(r_0 \in \Omega_j\). The corresponding source field is thus selected as

\[
(E^{src}, H^{src}) = \begin{cases} (E^{inc}, H^{inc}), & \text{in } \Omega_j \\
(0, 0), & \text{otherwise} \end{cases} \tag{10}
\]

for \(j = 1, 2\).

IV. SECOND-KIND INTEGRAL EQUATION FORMULATION

To approximate the unknown EM fields \((E_j, H_j), j = 1, 2\), we resort to a second-kind indirect Müller formulation. We start by introducing the off-surface integral operators

\[
(S_j \varphi)(r) := \int_{\Gamma} G_j (r, r') \varphi (r') \, ds'
\]

\[
+ \frac{1}{k_j^2} \nabla \times \int_{\Gamma} G_j (r, r') \nabla_j \cdot \varphi (r') \, ds'
\]

\[
(D_j \varphi)(r) := \nabla \times \int_{\Gamma} G_j (r, r') \nabla_j \varphi (r') \, ds'
\]

for \(r \in \mathbb{R}^3 \setminus \Gamma\), with \(\varphi\) being a vector field tangential to \(\Gamma\). (In what follows, the surface integrals over \(\Gamma\) must be interpreted as conditionally convergent.) The unknown EM fields \((E_j, H_j)\) are thus sought as

\[
E_j (r) := k_j^2 (S_j v(r) + i\omega \mu_j (D_j u)(r)) \tag{13a}
\]

\[
H_j (r) := k_j^2 (S_j u(r) - i\omega \varepsilon_j (D_j v)(r)) \tag{13b}
\]

for \(r \in \Omega_j, j = 1, 2\), in terms of unknown surface currents \(u\) and \(v\) that are to be determined by means of an SIE posed on \(\Gamma\). Clearly, the field defined in (13) satisfies Maxwell equations (2), in view of the fact that \(\nabla \times S_j = D_j\) and \(\nabla \times D_j = k_j^2 S_j\).

To derive an SIE for the currents, we make use of the well-known jump relations

\[
\hat{n} \times (S_j \varphi)|_{\pm} = T_j \varphi \quad \text{and} \quad \hat{n} \times (D_j \varphi)|_{\pm} = K_j \varphi \pm \frac{\varphi}{2} \tag{14}
\]

on \(r \in \Gamma\), where

\[
(T_j \varphi)(r) := \hat{n}(r) \times \int_{\Gamma} G_j (r, r') \varphi (r') \, ds' + \frac{1}{k_j^2} \hat{n}(r) \times \nabla \int_{\Gamma} G_j (r, r') \nabla_j \cdot \varphi (r') \, ds'
\]

and

\[
(K_j \varphi)(r) := \hat{n}(r) \times \nabla \times \int_{\Gamma} G_j (r, r') \varphi (r') \, ds'. \tag{16}
\]
Evaluating the integral representation formulae (13) on \( \Gamma \) and using (14), we obtain
\[
\mathbf{n} \times \mathbf{E}_j \mid_{\pm} = k_j^2 \mathbf{T}_j \mathbf{v} + i \omega \mu_j \left( \pm \frac{\mathbf{u}}{2} + \mathbf{K}_j \mathbf{u} \right) \quad (17a)
\]
for the electric fields, and
\[
\mathbf{n} \times \mathbf{H}_j \mid_{\pm} = k_j^2 \mathbf{T}_j \mathbf{u} - i \omega \varepsilon_j \left( \pm \frac{\mathbf{v}}{2} + \mathbf{K}_j \mathbf{v} \right) \quad (17b)
\]
for the magnetic fields. Therefore, enforcing the transmission conditions (4) by taking the appropriate linear combination of the relations (17), we arrive at the following SIE for the unknown vector of current densities \([\mathbf{u}, \mathbf{v}]^T\):
\[
\frac{i \omega}{2} \left[ \begin{pmatrix} (\mu_1 + \mu_2) \mathbf{u} \\ (\varepsilon_1 + \varepsilon_2) \mathbf{v} \end{pmatrix} + T \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \right] = \begin{pmatrix} M_{\text{sc}}^r \\ J_{\text{sc}}^r \end{pmatrix} \quad \text{on} \quad \Gamma \quad (18)
\]
where the block operator \( T \) is given by
\[
T = \begin{bmatrix} i \omega (\mu_2 \mathbf{K}_2 - \mu_1 \mathbf{K}_1) & k_j^2 \mathbf{T}_2 - k_j^2 \mathbf{T}_1 \\ k_j^2 \mathbf{T}_2^T - k_j^2 \mathbf{T}_1^T & -i \omega (\varepsilon_2 \mathbf{K}_2 - \varepsilon_1 \mathbf{K}_1) \end{bmatrix}. \quad (19)
\]

We emphasize that the rationale underlying expressing the EM fields as in (13) lies in making the singular operators \( \mathbf{T}_j \), \( j = 1, 2 \), appear in the resulting SIE (18) as the linear combination \( k_j^2 \mathbf{T}_2 - k_j^2 \mathbf{T}_1 \). Indeed, as shown in [44] and [32] and in Section VI below, this linear combination can be cast into a bounded integral kernel tractable by standard off-the-shelf quadrature rules.

Finally, it is worth mentioning that the two-layer media scattering problem considered in this section can as well be recast as the classical direct Müller integral equation involving the same operator \( T \), but with a different right-hand side that entails evaluation of the singular \( \mathbf{T}_j \) operator [26, Section 6.2].

V. Windowed Green Function Method

The fact that the SIE (18) is posed on an unbounded surface \( \Gamma \) introduces the salient issue of having to suitably truncate the computational domain to numerically approximate the SIE solution via MoM. Therefore, instead of solving (18) on the entire material interface \( \Gamma \), we make use of a windowed SIE to obtain approximations of the surface current densities \([\mathbf{u}, \mathbf{v}]^T\) over the relevant portion of \( \Gamma \) containing localized perturbations. To do so, we introduce a slow-rise infinitely smooth window function \( w_A : \mathbb{R}^3 \to \mathbb{R} \) which vanishes with all its derivatives outside the cylinder \( \{(x^2 + y^2)^{1/2} < A \} \times \mathbb{R} \).

More precisely, the window function is selected as \( w_A(x) = \eta((x^2 + y^2)^{1/2}, cA, A) \) for \( A > 0 \), \( 0 < c < 1 \), and
\[
\eta(s, s_0, s_1) := \begin{cases} 1, & \text{if } |s| < s_0 \\ \exp \left( \frac{2e^{-1/b}}{b - 1} \right), & \text{if } s_0 < |s| < s_1 \\ 0, & \text{if } |s| \geq s_1. \end{cases}
\]

The parameter value \( c = 0.7 \) is used in all the numerical examples presented in Section VII. (Other definitions of the window function, such as \( w_A(x) = \eta(x, cA, A)\eta(y, cA, A) \) or \( w_A(x) = \eta(x, cA_x, A_x)\eta(y, cA_y, A_y) \) with \( A_x, A_y > 0 \), for instance, can also be used as so to suitably adjust \( \Gamma_A \) to the particular shape of localized perturbations.)

We then consider the following windowed SIE:
\[
\frac{i \omega}{2} \left[ \begin{pmatrix} (\mu_1 + \mu_2) \mathbf{u} \\ (\varepsilon_1 + \varepsilon_2) \mathbf{v} \end{pmatrix} + T_A \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \right] = \begin{pmatrix} M_{\text{sc}}^r \\ J_{\text{sc}}^r \end{pmatrix} \quad \text{on} \quad \Gamma_A \quad (21)
\]
where \( \Gamma_A = \{ \mathbf{r} \in \Gamma : w_A(\mathbf{r}) \neq 0 \} \) and where the windowed operator \( T_A \) is defined as \( T \) in (19) but with the WGF
\[
G_{A,j}(\mathbf{r}, \mathbf{r}') = w_A(\mathbf{r}') G_j(\mathbf{r}, \mathbf{r}') \quad (22)
\]
replacing the free-space Green function \( G_j \) appearing in the definition of \( \mathbf{T}_j \) and \( \mathbf{K}_j \) in (15) and (16), respectively.

Existence and uniqueness of solutions of the windowed SIE (21) can be established (under reasonable smoothness assumptions on \( \Gamma_A \) and up to a countable set of frequencies \( \omega \)) by invoking the Fredholm alternative, which holds true in this case by virtue of the compactness of \( T_A \) (in an appropriate function space). Alternatively, for sufficiently small contrasts \( \varepsilon_1/\varepsilon_2 \) and \( \mu_1/\mu_2 \), existence and uniqueness could be established following a Neumann series approach.

As it turns out, \([\mathbf{u}_A, v_A]^T\) provides an excellent approximation of the exact currents \([\mathbf{u}, \mathbf{v}]^T\) within \( \Gamma_A \). Indeed, as in the 2-D EM case [24], [26], [28], [29], we have that the errors in the approximation \([\mathbf{u}_A, v_A]^T \approx [\mathbf{u}_A, v_A]^T \) decay super-algebraically fast in \( \Gamma_A \), for a fixed \( A > 0 \), as the window size \( A \) increases.

With the surface current densities \([\mathbf{u}_A, v_A]^T\) at hand, the approximate EM fields can be easily obtained by, respectively, substituting \( \mathbf{u} \) and \( \mathbf{v} \) by \( \mathbf{u}_A \) and \( v_A \) in the representation formula (13), and by replacing \( G_j \) by the WGF (22) in the off-surface operators \( \mathbf{S}_j \) and \( \mathbf{D}_j \) defined in (11) and (12), respectively. These substitutions produce the approximate fields
\[
\mathbf{\tilde{E}}_j(\mathbf{r}) := k_j^2 (\mathbf{S}_{A,j} v_A) (\mathbf{r}) + i \omega \mu_j (\mathbf{D}_{A,j} \mathbf{u}_A)(\mathbf{r}) \quad (23a)
\]
\[
\mathbf{\tilde{H}}_j(\mathbf{r}) := k_j^2 (\mathbf{S}_{A,j} \mathbf{u}_A) (\mathbf{r}) - i \omega \varepsilon_j (\mathbf{D}_{A,j} v_A)(\mathbf{r}) \quad (23b)
\]
for \( \mathbf{r} \in \Omega_j, \ j = 1, 2 \), where \( \mathbf{S}_{A,j} \) and \( \mathbf{D}_{A,j} \) are the resulting windowed off-surface operators.

We note that although formula (23) does not directly yield accurate far-fields, they can still be obtained from the accurate near-fields produced by (23) within \( \{ \mathbf{r} \in \mathbb{R}^3 : w_A(\mathbf{r}) = 1 \} \) in a manner akin to [24, Section 3.6] for the corresponding scalar problem (which in this case would involve the leading-order asymptotic approximation of the dyadic LGF, \( \mathbf{G}(\mathbf{r}, \mathbf{r}') \), as \( |\mathbf{r}| \to \infty \) [43, Section 2.6]).

As mentioned above, a limitation of the proposed approach is that first-kind SIEs, such as the PMCHWT formulation [33], [34], [35], which has been the preferred approach for EM transmission problems [45], is not directly compatible with the WGF approach. In a nutshell, windowed kernels decay exponential fast near the edges of the truncated surface, thus allowing surface currents near those edges to lie in the approximate nullspace of the PMCHWT WGF-MoM matrices. Such matrices have then eigenvalues very close to the origin making the linear system too ill-conditioned to be accurately solved by either direct or iterative method. In contrast, second-kind SIEs, like the ones used in this contribution, do not
suffer from this problem because the identity term shifts the spectrum sufficiently far away from the origin (see Fig. 4 in Section VII-B). A possible remedy to this issue is the use of Calderón preconditioners [36], which take advantage of the operators’ self-regularizing properties to convert first-kind SIEs into equivalent well-conditioned second-kind SIEs.

VI. MoM DISCRETIZATION

We start off this section by considering a triangulation of the truncated surface \( \Gamma_A \) which lies within the support of the window function \( \omega_A \). We then expand \([u_A, v_A]^{\top}\) in terms of the standard div-conforming RWG basis functions [46]. In detail, we let

\[
    u_A(r) \approx \sum_{n=1}^{N} u_n f_n(r) \quad \text{and} \quad v_A(r) \approx \sum_{n=1}^{N} v_n f_n(r) \tag{24}
\]

for \( r \in \Gamma_A \), where \( N \) is the total number of edges in the triangular mesh, and \( f_n \) are the RWG basis functions [47].

As in [44], we apply the Galerkin scheme to determine the coefficients \( u_n \) and \( v_n \) in the approximations (24) by replacing (24) in the windowed SIE (21) and then testing the resulting equations against the same div-conforming basis functions \( f_n \). We thus obtain the following linear system for the coefficients:

\[
    Mx = b \tag{25}
\]

where \( x = [u_1, \ldots, u_N, v_1, \ldots, v_N]^{\top} \in \mathbb{C}^{2N} \)

\[
    M = \begin{bmatrix} M^{(1,1)} & M^{(1,2)} \\ M^{(2,1)} & M^{(2,2)} \end{bmatrix} \in \mathbb{C}^{2N \times 2N} \tag{26}
\]

with blocks \( M^{(p,q)} \), \( p, q = 1, 2 \) defined as

\[
    M^{(p,q)} = \int_{\Gamma_A} f_m(r) \cdot (M^{(p,q)} f_n)(r) \, ds, \quad n, m = 1, \ldots, N
\]

in terms of the operators

\[
    M^{(1,1)} \varphi = -\frac{i\omega (\mu_1 + \mu_2)}{2} \varphi + i\omega (\mu_2 K_{A,2} - \mu_1 K_{A,1}) \varphi,
\]

\[
    M^{(1,2)} \varphi = M^{(2,1)} \varphi = (k_2^2 T_{A,2} - k_1^2 T_{A,1}) \varphi,
\]

\[
    M^{(2,2)} \varphi = \frac{i\omega (\epsilon_1 + \epsilon_2)}{2} \varphi + i\omega (\epsilon_1 K_{A,1} - \epsilon_2 K_{A,2}) \varphi.
\]

On the other hand, the right-hand side vector \( b \in \mathbb{C}^{2N} \) is given by

\[
    b_m = \int_{\Gamma_A} f_m(r) \cdot M^{\text{sc}} \, ds, \quad m = 1, \ldots, N,
\]

and \( b_m = \int_{\Gamma_A} f_m(r) \cdot J^{\text{sc}} \, ds, \quad m = N + 1, \ldots, 2N \).

Evaluation of the matrix entries boils down to compute integrals of the form

\[
    I^{(1)}_{m,n} = \int_{\Gamma_A} f_m(r) \cdot \left( \hat{n}(r) \times \nabla \times \int_{\Gamma_A} G_{A,j}(r, r') f_n(r') \, ds' \right) \, ds \tag{27}
\]

in the case of diagonal blocks \( M^{(1,1)} \) and \( M^{(2,2)} \), and integrals of the form

\[
    I^{(2)}_{m,n} = \int_{\Gamma_A} f_m(r) \cdot \left( \hat{n}(r) \times \int_{\Gamma_A} G_{A,j}(r, r') f_n(r') \, ds' \right) \, ds
\]

\[
    I^{(3)}_{m,n} = \int_{\Gamma_A} f_m(r) \cdot \left( \hat{n}(r) \times \int_{\Gamma_A} \nabla[G_{A,2}(r, r') - G_{A,1}(r, r')] \nabla' \cdot f_n(r') \, ds' \right) \, ds
\]

in the case of off-diagonal blocks \( M^{(1,2)} \) and \( M^{(2,1)} \), where \( G_{A,j}, \ j = 1, 2 \), are defined in (22). Note that the integrands above become singular whenever the supports of \( f_m \) and \( f_n \) intersect each other. However, given that

\[
    \nabla[G_{2}(r, r') - G_{1}(r, r')] = -\frac{(k_2^2 - k_1^2)}{2} \frac{(r - r')}{|r - r'|^2} + o(1)
\]

as \( |r - r'| \to 0 \), we have that the integrand in the definition of \( I^{(3)}_{m,n} \) remains bounded. In the numerical examples considered in the next section, we use the Duffy-like singularity cancellation technique presented in [48] to render these weakly singular integrands into smooth functions that we integrate by means of standard Gauss quadrature rules.

Finally, we briefly discuss the selection of the parameter \( A \) and the mesh size \( h \) associated with the discretization of \( \Gamma_A \).

Since the WGF truncation errors in \( T_{A,j} \) and \( K_{A,j} \), \( j = 1, 2 \), decay faster than any power of \(|k_j A|^{-1}\) as \( A \) increases [26], \( A \) should be selected such that \( A > \max\{|k_1^{-1}, |k_2^{-1} \}| \). It was found in practice that \( A > 16 \pi \max\{|k_1^{-1}, |k_2^{-1} \} + R \), where \( R > 0 \) is the radius of the smallest ball containing the perturbations, is more than enough to suppress any error stemming from the windowing approximation, making the overall WGF-MoM error of order \( O(h^2) \) for any reasonable small mesh size \( h \) (see Figs. 2 and 3). Regarding the discretization of \( \Gamma_A \), on the other hand, it has to be such that the spatial oscillations of the surface integrands in the integral operators are well-resolved, i.e., \( h < \pi \max\{|k_1^{-1}, |k_2^{-1} \} \) so that the Nyquist criterion is not violated.

VII. VALIDATION AND EXAMPLES

A variety of numerical examples are presented in this section to validate and demonstrate the accuracy, efficiency, and applicability of the proposed methodology.

A. PEC Hemispherical Bump

First, to validate the proposed WGF-MoM approach, we consider the problem of scattering of an incident EM plane wave (6) of wavelength \( \lambda = 2\pi/k_1 = 1 \), by a PEC...
hemispherical bump of radius \( \lambda \) placed on top of the PEC half-space \( (z < 0) \) (see inset in Fig. 2). We thus compare the exact solution \( \mathbf{E}^{\text{ref}} \) (see Appendix A) with the numerical WGF-MoM solution, which is obtained using an indirect windowed MFIE formulation. We note that since the exact PEC half-space Green function can be computed in closed form (via the method of images), this and more general PEC obstacle and bump-like scattering problems can be directly cast into the classical MFIE and EFIE posed on the obstacle/bump’s surface. There is therefore no particular advantage of using the WGF method in these cases. The reason why this problem is here considered is that to the best of the authors’ knowledge, this is the only problem of scattering by a locally perturbed infinite planar surface that admits an exact Mie series solution.

In detail, the approximate total electric field takes the form \( \mathbf{E}^{\text{tot}} = \mathbf{E}^{E} + \mathbf{E}^{\text{inc}} \), where \( \mathbf{E}^{\text{inc}} \) is given in Section III and \( \mathbf{E}^{E} = \mathbf{D}_{A,1}[u_A] \) with the currents \( u_A \) being the solution of the windowed MFIE

\[
\frac{u_A}{2} + \mathbf{K}_{A,1}[u_A] = -\hat{n} \times \mathbf{E}^{\text{inc}} \quad \text{on} \quad \Gamma_A
\]

which is solved using the standard MoM discretization [47]. (The corresponding total magnetic field can be retrieved from \( u_A \) via \( \mathbf{H}^{\text{tot}} = \mathbf{H}^{E} + \mathbf{H}^{\text{inc}} \) with \( \mathbf{H}^{E} = -i\omega \mathbf{E}^{\text{inc}} \)).

Fig. 2 displays the electric field errors

\[
\text{error} = \max_{r \in \Theta} |\mathbf{E}^{\text{tot}}(r) - \mathbf{E}^{\text{ref}}(r)| / \max_{r \in \Theta} |\mathbf{E}^{\text{ref}}(r)| \quad (27)
\]

obtained by evaluating both the solutions at a fixed target point set \( \Theta \) on a hemispherical surface of radius \( 2\lambda \) concentric to the PEC bump, for various meshes \( (h > 0) \) and window \( (A > 0) \) sizes. The TE- and TM-polarized plane wave incident fields (6) at the grazing angle \( \pi/32 = \arctan(k_z/k_y) \) were used in these examples. The respective linear systems (25) were iteratively solved by means of GMRES [49] which converged in about 20 iterations using a relative tolerance of \( 10^{-5} \) and the Jacobi (diagonal) preconditioner. Almost identical results are obtained for incidences closer to normal.

There are two types of errors present in these results, the error stemming from the WGF approximation, which decreases super-algebraically as \( A \to \infty \), and the MoM error, which decreases as \( h^2 \) as \( h \to 0 \). The former becomes dominant for small \( A \) values, as can be seen in the flattening of the error curves for small \( h \) values, while the latter becomes dominant for sufficiently large \( A \) values, as can be seen in the quadratic error decay as \( h \) decreases. These results validate the convergence of our windowed MoM solver, which is not affected by the planewave incidence angle and polarization.

We mention in passing that this simple windowed MFIE formulation can as well be used to tackle the rather classical PEC open cavity problem (cf. [10, Ch. 10]). The standard SIE formulations for this problem [23], [50], [51] entail introducing an artificial transparent surface to close the open cavity, which is not needed by the windowed MFIE formulation.

B. Sommerfeld Half-Space Problem

Our next example deals with the classical Sommerfeld half-space problem [1]. We consider an incident electric field \( \mathbf{E}^{\text{inc}} \) produced by the superposition of ten randomly placed (at the points \( r_\ell, \ell = 1, \ldots, 10 \)) electric dipole sources (8). The dipole sources are uniformly distributed within the boundaries of a cylinder of radius \( \lambda \), height \( 2\lambda \), and centered at \((0, 0, 2\lambda)\) (see inset in Fig. 3), where \( \lambda = 2\pi/k_1 = 1 \) m in this case. The incident field impinges on a dielectric half-space \( \Omega_2 = \{z < 0\} \) with \( k_2 = (2)^{1/2}k_1 \) \( (\varepsilon_2 = 2\varepsilon_1) \). The exact total electric field takes the form \( \mathbf{E}^{\text{ref}}(r) = \sum_{\ell=1}^{10} \mathbf{G}(r, r_\ell) p_\ell \) where \( \mathbf{G} \) is the dyadic LGF [43], and \( p_\ell, \ell = 1, \ldots, 10 \), are the random polarization unit vectors.

The approximate total electric field, on the other hand, is given by \( \mathbf{E}^{\text{tot}} = \mathbf{E}_1 + \mathbf{E}^{\text{inc}} \) in \( \Omega_1 \), where \( \mathbf{E}_1 \) is obtained from (23a) with currents \( (u_A, v_A) \) produced by means of MoM applied to the windowed SIE (21), and where the source field \( \mathbf{E}^{\text{inc}} \) is given in (10).

Fig. 3 displays the errors (27) in the total field \( \mathbf{E}^{\text{tot}} \) for various meshes and window sizes. The target point set \( \Theta \) used to compute the errors encompasses 2332 points lying on the surface of the cylinder containing the dipole sources (see inset in Fig. 3). The reference (total) field in this example was produced by the LGF FORTRAN code [40]. The particular source–target point configuration of Fig. 3 intentionally avoids dealing with difficult cases that could affect the accuracy of LGF evaluations.

Once again, fast convergence is observed as the window size \( A > 0 \) increases while the expected second-order convergence is attained as the mesh size \( h > 0 \) decreases. The smallest errors reported in Fig. 3 (for \( h \approx 0.1 \)) are reproduced in Table I for various window sizes used in this example. In view of the fact that the log–log slope \( \sigma_h \) grows (in magnitude) as \( A \) increases, we have that the error decays super-algebraically fast as \( A \) increases (algebraic convergence of any fixed order would produce an approximately constant slope \( \sigma_h \)).

Interestingly, as in the PEC hemispherical bump example and in all the examples presented in this work, the Jacobi diagonal preconditioner significantly reduces the number of...
TABLE I
ERRORS IN FIG. 3 FOR THE SEVEN WINDOW SIZES A USED, WHICH ARE INDEXED BY n = 1, . . . , 7, CORRESPONDING TO h ≈ 0.1. THE LOG–LOG SLOPE OF THE ERROR (AS A FUNCTION OF 1A) IS COMPUTED AS

\[ \sigma_n = -\log(|\text{error}_n|/|\text{error}_{n-1}|) / \log(A_n/A_{n-1}) \]

FOR n = 2, . . . , 7.

INCREASING \( \sigma_n \) VALUES FOR n ≥ 4 DEMONSTRATE THE SUPER-ALGEBRAIC CONVERGENCE OF THE WGF-MoM ALGEBRAIC LINEAR SYSTEM (25). TO EXAMINE GMRES ITERATIONS REQUIRED TO APPROXIMATELY SOLVE THE RESULTING SYSTEMS, WE OBTAINED THE SPECTRA OF THE NON-PRECONDITIONED AND THE JACOBI-DIAGONALLY PRECONDITIONED MATRICES (TOP) AND (BOTTOM) FOR THE SOLUTION OF THE SOMMERFELD SIE SYSTEM CONSISTING OF A MFIE BLOCK THAT ENFORCES THE PEC BOUNDARY ε, AND A DIFEIE BLOCK THAT ACCOUNTS FOR THE TRANSMISSION CONDITION AT THE PLANAR DIELECTRIC INTERFACE \( \Gamma \).

GMRES iterations required to approximately solve the resulting WGF-MoM algebraic linear system (25). To examine this fact in more detail, we present Fig. 4 which shows the eigenvalues of the non-preconditioned and the Jacobi-diagonally preconditioned matrices corresponding to the Sommerfeld dipole problem using window sizes \( A = 3\lambda \) (top) and \( A = 6\lambda \) (bottom).

Fig. 4. Eigenvalues of the WGF-MoM matrices (26) (left) and corresponding diagonally preconditioned matrices (right) for the solution of the Sommerfeld half-space problem of Section VII-B using \( A = 3\lambda \) (top) and \( A = 6\lambda \) (bottom).
are much smaller, of dimensions NS
one free-space Green function evaluation costs significantly
between the two methods is mainly explained by the fact that
the cost associated with enforcing the transmission conditions
is directly evaluated via numerical integration techniques). It is
used (that difference is orders of magnitude larger when LGF
less than one LGF evaluation, even when efficient DCIM is
considered. For instance, structures having several flat layers
possess remarkable advantages over the WGF approach in
certain cases. Despite the above-mentioned drawbacks, the LGF-based SIEs
can be easily handled by LGF at almost no additional cost,
whereas the WGF approach requires the use of additional
surface currents at each one of the interfaces, even when they
do not contain any perturbation. Similarly, problems involving
moderate numbers of small-area inclusions entail few LGF
evaluations, and hence can be easily treded by this approach.

D. Cavity in a Dielectric Half-Space

Next, we consider the problem of scattering of a TE-polarized planewave (6) that impinges on a spherical cavity in a dielectric half-space, produced by the proposed WGF-MoM with A = 8.5λ. Truncated surface (gray) and field view on
(a) yz-plane, (b) yz-plane, and (c) xy-plane within the region \{w_A(r) = 1\}.

An even better relative performance of WGF-MoM is expected when considering, for instance, structures having localized surface perturbations, like the ones considered in Section VII-D and VII-E, which are particularly cumbersome to deal with the LGF-based methods. In this case, the enforcement of the continuity of the total tangential electric and magnetic fields at dielectric interfaces entails evaluation not only of the dyadic LGF itself but also of its curl, further affecting the overall performance of LGF-MoMs. Moreover, in such cases the evaluation of LGF is hindered by the lack of exponential decay of the spectral LGF when both the source and target points lie on the interface between two layers. Despite the above-mentioned drawbacks, the LGF-based SIEs possess remarkable advantages over the WGF approach in certain cases. For instance, structures having several flat layers
almost identical number of GMRES iterations were needed to achieve the same accuracy occurring outside $\{|w_A(r)| = 1\}$ is clearly observed in those figures, especially near the interface $\Gamma$. In particular, this example shows that the WGF-MoM does not directly produce correct near-fields. As mentioned in Section V, a simple remedy to this problem is to map the correct near-fields, produced by WGF-MoM, to the far-field. This can be done by means of the Stratton–Chu formula based on LGF integrating over a surface enclosing the perturbation, and then replacing the kernels by their leading-term asymptotic expansion as $|r| \to \infty$.

E. All-Silica Metasurface

Our next example presents the full 3-D solution of a problem of scattering by an all-silica (SiO$_2$) metasurface (cf. [52]) consisting of an array of $10 \times 10$ nano-rods of subwavelength radii, ranging from 36.7 to 77.5 nm, and a fixed height of 364 nm, which is illuminated from $\Omega_2$ by a normally incident plane EM wave (6) with $p = (1, 1, 1)$ and $k = k_2(0, 0, 1)$. Fig. 8(a) displays the surface $\Gamma_A$ used in this example, where the window size $A = 6\lambda = 3.9 \ \mu m$ ($\lambda = 650 \ nm$) is used. (The nano-rods are shown in various colors for visualization purposes.) The nano-rod radii follow a parabolic profile that effectively steers the direction of the transmitted light by controlling the phase change as it penetrates $\Gamma_A$, thus achieving the focusing effect demonstrated in Fig. 8(b) and (c), which displays the electric field intensity at surfaces parallel to the $yz$- and $xy$-planes, respectively. The surface mesh used in this example, which was properly refined so as to account for the numerous small-scale features, comprised a total of 17822 nodes and 53335 edges. The corresponding SIE solution was produced using a Jacobi-preconditioned GMRES solver, which converged in 45 iterations to a tolerance of $10^{-4}$. Our (unaccelerated) FORTRAN OpenMP-parallelized WGF-MoM implementation took $\sim 65 \ min$ in constructing the system matrix, $\sim 15 \ min$ in solving the linear system, and $\sim 35 \ min$ in producing the high-fidelity fields shown in Fig. 8 using a workstation with 48 cores (96 threads, dual Xeon Gold 6240R) and 500 GB of memory.

F. Plasmonic Solar Cell

In the last example of this article, we consider a plasmonic solar cell structure [53] consisting of ten gold nanoparticles of diameter 100 nm lying on top of a 500-nm-thick silicon nitride (Si$_3$N$_4$) film backed by a silicon (Si) substrate [see Fig. 9(a)]. The structure is illuminated by a normally incident plane wave (6) coming from above at $\lambda = 572 \ nm$ and polarized according to $p = (1, 1, 1)$. The total electric field intensity $|E_{\text{tot}}|^2$ produced by the proposed WGF-MoM is shown in Fig. 9. The frequency used in this example excites plasmon resonances in the metallic nanoparticles leading to a strong local field enhancement around the metallic nanoparticles [8], as can be observed in the zoomed inset figure in Fig. 9(b).

The presence of multiple penetrable interfaces made it necessary to generalize the SIE formulation presented above...
in Section IV. In detail, letting $\Omega_1$, $\Omega_2$, $\Omega_3$, and $\Omega_4$ denote the subdomains occupied by air ($\epsilon_1 = \epsilon_0$), silicon nitride ($\epsilon_2 = 2.0483\epsilon_0$), silicon ($\epsilon_3 = (4.0191 + 0.031373i)\epsilon_0$), and gold nanoparticles ($\epsilon_4 = (0.33221 + 2.74i)\epsilon_0$), respectively, we express the EM fields $\mathbf{E}_j, \mathbf{H}_j$ in $\Omega_j$ as in (13) but in terms of the off-surface operators $S_j$ (11) and $D_j$ (12) defined by integrals over $\partial\Omega_j$, $j = 1, \ldots, 4$. Enforcing then the continuity of the total tangential fields $\mathbf{n} \times (\mathbf{E}_j + \mathbf{E}^{sc}, \mathbf{H}_j + \mathbf{H}^{sc})$ at each of the interfaces $\partial\Omega_j$, using as source field $(\mathbf{E}^{sc}, \mathbf{H}^{sc})$ the total EM field solution of the problem of scattering by the three-layer structure (without the nanoparticles) (see [43, Section 2.1.3]), we arrive at a $3 \times 3$ block second-kind SIE system that is windowed and discretized using the MoM presented in Section VI. The approximate total fields $(\mathbf{E}^{tot}, \mathbf{H}^{tot}) = (\mathbf{E}_0 + \mathbf{E}^{sc}, \mathbf{H}_0 + \mathbf{H}^{sc})$, $j = 1, \ldots, 4$, are retrieved by windowing the corresponding field representation formula.

The two planar triangular meshes used in this example comprise 35 785 edges each, while the total number of edges in the spherical meshes amounted to 11 337. The planar meshes were suitably refined near the bottom tip of the spheres to properly account for possible nearly singular integration issues. The linear system was solved by means of GMRES, which converged in 28 iterations to the prescribed tolerance ($10^{-4}$). The overall time needed by our OpenMP-parallelized WGF-MoM implementation to produce the three plots of $|\mathbf{E}^{tot}|^2$ presented in Fig. 9, on the horizontal planes at $z = 50$ nm and $z = -250$ nm in (b) and (c), respectively, as well as on the vertical plane $\{x = 0\}$ in (a), was around 64 min on the aforementioned 48-core machine.

This article presents an SIE method for EM scattering by locally perturbed planar layered media. The proposed methodology, which extends the WGF method put forth in [24], [25], and [26] for the (scalar) Helmholtz equation, does not entail evaluation of any Sommerfeld integrals thus avoiding their inherent costs and challenges that they pose, but at the expense of adding new unknowns on the planar interfaces and requiring a larger linear system that must be solved. The method leverages an indirect second-kind Müller SIE formulation featuring weakly singular integral operators expressed in terms of free-space Green functions. Upon windowing the integral kernels and applying a standard Galerkin MoM discretization based on RWG basis functions, well-conditioned linear systems amenable to be solved iteratively by GMRES are obtained. The resulting methodology exhibits both second-order convergence (in the near-fields) as the mesh size is decreased and high-order convergence (super-algebraic) as the window size is increased, as demonstrated by a thorough set of comparative examples. A number of challenging problems including scattering by cavities, metasurfaces, and plasmonic solar cell structures further validate and showcase the capabilities of the proposed WGF-MoM. It is worth mentioning, however, that larger-scale and more realistic metasurface and solar cells configurations than the ones considered here inevitably require use of fast algorithms such as the fast multipole method [54] or $\mathcal{H}$-matrices [55].

This work certainly opens up a number of possible follow-up research directions. For example, an accurate SIE solver capable of handling more general metasurface designs requires proper handling of multimaterial junctions. As in the 2-D case [56], [57], this could be accomplished within our 3-D WGF-MoM framework using a second-kind single-trace formulation [58]. The robust low-frequency behavior of Müller’s formulation reported in [44], on the other hand, brings about the idea of extending the proposed methodology to the time domain by suitably combining it with the convolution quadrature schemes, as was done in the 2-D case in [30].

APPENDIX A
HEMISPHERICAL BUMP PROBLEM: MIE SERIES SOLUTION

We here make use of the classical Mie series solution and the theory of images, to produce the exact solution of the problem of scattering of a plane EM wave by a hemispherical PEC bump on top of a PEC half-space. Consider an incident plane EM wave, with grazing angle $\alpha$, given by

$$
\mathbf{E}_{inc}(r) = E_0 e^{ik(y \cos \alpha - z \sin \alpha)} \begin{cases} 
\hat{x}, & \text{if TE polarized} \\
\hat{y} \sin \alpha + \hat{z} \cos \alpha, & \text{if TM polarized}
\end{cases}
$$

Using the theory of images we have that the resulting total EM field, which satisfies $\mathbf{n} \times \mathbf{E}^{tot} = \mathbf{0}$ on $\Gamma$, can be expressed as

$$
\mathbf{E}^{tot} = \mathbf{E}_{inc}^{tot} + \mathbf{E}^{Mie} + \mathbf{E}_{inc}^{Mie}
$$

where $\mathbf{E}^{Mie}$ is the Mie's series solution.
where \[ \mathbf{E}^{inc} = -\mathbf{E}^{inc}_{r}, \] if TE polarized
and \[ \mathbf{E}^{Mie} \] and \[ \mathbf{E}^{Mie} \] are the well-known Mie series solution of the problem of scattering of an entire PEC sphere, with the same radius as the bump, by \[ \mathbf{E}^{inc} \] and \[ \mathbf{E}^{inc} \], respectively.

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