

Communication

A Multitrace Surface Integral Equation Solver to Simulate Graphene-Based Devices

Ran Zhao¹, Liang Chen¹, Ping Li¹, Jun Hu¹, and Hakan Bagci²

Abstract—A multitrace surface integral equation (MT-SIE) solver is proposed to analyze electromagnetic field interactions on composite devices involving magnetized and nonmagnetized graphene sheets. The computation domain is decomposed into two subdomains: an exterior subdomain that represents the unbounded background medium where the device resides in an interior subdomain that represents the dielectric substrate. Resistive Robin transmission conditions (RRTCs) are formulated to describe the infinitesimally thin graphene sheet that partially covers the surface between the two subdomains. On the rest of this surface, traditional Robin transmission conditions (RTCs) are enforced. The electric and magnetic field equations are used as the governing equations in each subdomain. The governing equations of a subdomain are locally coupled to the governing equations of its neighbor using RRTCs and RTCs. The accuracy and the applicability of the proposed MT-SIE solver are demonstrated by various numerical examples.

Index Terms—Graphene-based device, multitrace (MT), resistive boundary condition (RBC), surface integral equation (SIE).

I. INTRODUCTION

Graphene is a 2-D material with remarkable electrical, mechanical, and thermal properties [1]. Its surface conductivity depends on temperature T , chemical potential (Fermi level) μ_c , and particle scattering rate Γ , and therefore it can be dynamically tuned to manipulate electromagnetic fields. This has led to the development of various graphene-based devices such as thin-film transistors [2], gas sensors [3], solar cells [4], and photonic modulators [5]. In addition, a graphene sheet can be biased using a static magnetic field (which makes its conductivity a tensor), increasing its tunability even more. Magnetized graphene has been used in the design of various tunable electromagnetic devices operating in the different bands changing from microwave to terahertz (THz) frequencies. Some examples of these devices are tunable filters [6], phase shifters [7], reconfigurable THz antennas [8], [9], and frequency-selective surfaces [10].

For almost all of the devices listed above, a graphene sheet is located on a dielectric substrate and its thickness is several orders

smaller than any other device dimension. To simulate such a device, one can directly discretize the graphene sheet using volumetric elements but this yields a multiscale mesh with a large number of elements [11]. Furthermore, the resulting matrix system is often ill-conditioned [12], [13]. These bottlenecks can be circumvented by replacing the graphene sheet with an infinitesimally thin surface and enforcing resistive boundary conditions (RBCs) on it [14]–[17]. This approach has been incorporated within finite-difference time-domain method [14], [15] and discontinuous Galerkin time-domain scheme [16], [17], and the resulting solvers have been used to simulate various graphene-based devices. Although these differential equation solvers are versatile in handling geometrically complicated devices, they use a volumetric mesh in the whole computation domain and have to use domain truncation techniques (such as absorbing boundary conditions or perfectly matched layers) and consequently become computationally demanding especially when they are used to simulate large-scale problems.

These bottlenecks can be addressed by switching to an integral equation-based formulation. In [18] and [19], electromagnetic field interactions on a graphene sheet are first formulated in the form of a volume integral equation. Then, this equation is “reduced” into surface integral equations (SIEs) under the thin dielectric sheet approximation [20]. In [21] and [22], an equivalent circuit model is obtained for the graphene sheet using an electric field integral equation, then this model is incorporated into the partial element equivalent circuit method [23]. In [24] and [25], a magnetic field integral equation is solved to analyze electromagnetic scattering from graphene disks and strips that reside in an unbounded medium. None of these integral equation-based approaches deal with the case when a graphene sheet is located on a dielectric substrate.

To address this shortcoming, in [26] and [27], RBCs representing the graphene sheet are solved together with the Poggio–Miller–Chang–Harrington–Wu–Tsai integral equation [28] enforced on the surfaces of the dielectric substrate. These two schemes completely avoid volumetric meshes. However, for geometrically complicated devices, the matrix system obtained by discretizing this coupled system of SIEs with the Rao–Wilton–Glisson (RWG) functions [29] becomes ill-conditioned. This degrades the accuracy and the efficiency of the solvers, especially for electrically-large devices.

In recent years, integral-equation domain-decomposition methods that make use of multitrace SIEs (MT-SIEs) and Robin transmission conditions (RTCs) have found widespread use in the electromagnetic simulation of a wide range of structures changing from penetrable objects to large cavities, composite objects, and so on [30]–[34]. These methods decompose the computation domain into subdomains and enforce SIEs on their (internal) surfaces. Then, SIEs of a given subdomain are “coupled” to SIEs of its neighbors via RTCs. This local-coupling approach improves the scalability and robustness of the traditional “single-domain” SIE solvers and is more suitable for solving large-scale problems.

In this work, an MT-SIE solver is proposed to simulate electromagnetic field interactions on graphene-based devices. The graphene sheet that is located on the surface between the unbounded

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background medium and the dielectric substrate is described by RBCs. Resistive RTCs (RRTC) are formulated to incorporate these RBCs within the MT-SIE formulation. The computation domain is decomposed into two subdomains: an exterior subdomain that represents the unbounded background medium where the device resides in an interior domain that represents the dielectric substrate. The electric and magnetic field equations are used as the governing equations in each subdomain. These subdomain SIEs are coupled to each other using RRTC (that represent the graphene) and “traditional” RTCs (that represent the tangential electric and magnetic field continuity). Note that RBCs and corresponding RRTC can account for both nonmagnetized graphene (with a scalar conductivity) and magnetized graphene (with a tensor anisotropic conductivity). Compared to the differential equation solvers [12]–[17], the proposed MT-SIE solver avoids volumetric meshes and does not require absorbing boundary conditions. Compared to the SIE solvers developed to simulate only graphene sheets [18], [19], [21], [22], [24], [25], the proposed MT-SIE solver accounts for the dielectric substrate. Furthermore, it inherits all advantages of the MT-SIE solvers developed to simulate composite objects [32]–[34]. It yields a matrix system that can be efficiently solved using an iterative solver even for electrically large devices and allows for higher flexibility in mesh generation for multilayered substrates. Also, note that the formulation proposed in this work can easily be extended for simulation of various devices making use of other 2-D materials and to account for generalized sheet transmission conditions (GSTCs) formulated using (anisotropic) polarization susceptibilities [35], [36].

The rest of this communication is organized as follows. In Section II, first, the surface conductivity of the nonmagnetized and magnetized graphene sheets is provided. This is followed by the derivation of RRTC for the graphene sheet. Then, MT-SIEs underlying the proposed solver are derived, and the matrix system resulting from their RWG-based discretization is provided. Section III provides numerical examples to demonstrate the accuracy and the applicability of the proposed solver. Conclusions are summarized in Section IV.

II. FORMULATION

In this section, first, RBCs representing magnetized and nonmagnetized graphene sheets are provided. Then, RRTC pertinent to these RBCs are derived. This is followed by the detailed mathematical description of the MT-SIE solver developed to simulate graphene-based devices. Note that for the sake of brevity in notation, the dependence on space (i.e., location vector \mathbf{r}) is omitted for all variables used in this section.

A. RBCs and RRTC for Graphene Sheets

The graphene sheet is modeled as a zero-thickness surface with conductivity $\overline{\sigma}_g$. RBCs on this surface are expressed as [24]

$$\hat{\mathbf{n}}_1 \times (\mathbf{E}_1 - \mathbf{E}_2) = 0 \quad (1)$$

$$\hat{\mathbf{n}}_1 \times (\mathbf{H}_1 - \mathbf{H}_2) = -\frac{1}{2} \overline{\sigma}_g \cdot [\hat{\mathbf{n}}_1 \times \hat{\mathbf{n}}_1 \times (\mathbf{E}_1 + \mathbf{E}_2)] \quad (2)$$

where $\{\mathbf{E}_1, \mathbf{H}_1\}$ and $\{\mathbf{E}_2, \mathbf{H}_2\}$ are the electromagnetic fields on the two sides of the graphene surface and $\hat{\mathbf{n}}_1$ is this surface’s unit normal vector pointing into side 1.

Assume the graphene sheet is located on the xy -plane and a static magnetic field with flux $\mathbf{B} = \hat{\mathbf{z}}B_0$ “biases” the graphene sheet. In this case, the surface conductivity $\overline{\sigma}_g$ is given by Hanson [37]

$$\overline{\sigma}_g = \begin{bmatrix} \sigma_{xx} & -\sigma_{yx} & 0 \\ \sigma_{yx} & \sigma_{xx} & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (3)$$

where σ_{xx} and σ_{yx} are approximated by a Drude-like models as

$$\sigma_{xx} = \sigma_0 \frac{1 + j\omega\tau}{(\omega_c\tau)^2 + (1 + j\omega\tau)^2} \quad (4)$$

$$\sigma_{yx} = \sigma_0 \frac{\omega_c\tau}{(\omega_c\tau)^2 + (1 + j\omega\tau)^2}. \quad (5)$$

Here, ω is the frequency, τ is the scattering time, $\omega_c \approx eB_0v_F^2/\mu_c$ is the cyclotron frequency, $v_F \approx 10^6 \text{ m} \cdot \text{s}^{-1}$ is the Fermi velocity, e is the electron charge, μ_c is the chemical potential

$$\sigma_0 = \frac{e^2\tau k_B T}{\pi\hbar^2} \left[\frac{\mu_c}{k_B T} + 2 \ln \left(e^{-\mu_c/k_B T} + 1 \right) \right] \quad (6)$$

k_B is the Boltzmann’s constant, $T = 300 \text{ K}$ is the temperature, and \hbar is the reduced Planck’s constant.

If the graphene sheet is not biased by a magnetic field, the surface conductivity $\overline{\sigma}_g$ reduces to a scalar and is expressed using the Kubo formula [38]: $\sigma_g = \sigma_{\text{intra}} + \sigma_{\text{inter}}$. Here, the intraband and interband contributions σ_{intra} and σ_{inter} are given by

$$\sigma_{\text{intra}} = \frac{2e^2 k_B T}{\pi\hbar} \frac{1}{\hbar} \ln \left[2 \cosh \left[\frac{\mu_c}{2k_B T} \right] \right] \frac{-j}{\omega - j\tau^{-1}} \quad (7)$$

$$\sigma_{\text{inter}} = \frac{e^2}{4\hbar} \left(H \left(\frac{\omega}{2} \right) - j \frac{4\omega}{\pi} \int_0^\infty \frac{H(\varepsilon) - H(\omega/2)}{\omega^2 - 4\varepsilon^2} d\varepsilon \right) \quad (8)$$

where function $H(\varepsilon)$ is defined as

$$H(\varepsilon) = \frac{\sinh(\hbar\varepsilon/k_B T)}{\cosh(\mu_c/k_B T) + \cosh(\hbar\varepsilon/k_B T)}. \quad (9)$$

Note that in the rest of this section, the general case of a tensor-valued surface conductivity is assumed.

For traditional domain-decomposition formulations, RTCs are used to ensure the continuity of the electromagnetic fields on two sides of a surface that divides a domain into subdomains [39]. These traditional RTCs are given by Peng *et al.* [30]

$$\begin{aligned} \mathbf{J}_1 - \hat{\mathbf{n}}_1 \times \mathbf{M}_1 + \mathbf{J}_2 + \hat{\mathbf{n}}_2 \times \mathbf{M}_2 &= 0 \\ \hat{\mathbf{n}}_1 \times \mathbf{J}_1 + \mathbf{M}_1 - \hat{\mathbf{n}}_2 \times \mathbf{J}_2 + \mathbf{M}_2 &= 0. \end{aligned} \quad (10)$$

Here, $\mathbf{J}_1 = \hat{\mathbf{n}}_1 \times \mathbf{H}_1$, $\mathbf{J}_2 = \hat{\mathbf{n}}_2 \times \mathbf{H}_2$, $\mathbf{M}_1 = -\hat{\mathbf{n}}_1 \times \mathbf{E}_1$, $\mathbf{M}_2 = -\hat{\mathbf{n}}_2 \times \mathbf{E}_2$, and $\hat{\mathbf{n}}_2$ is the unit normal vector pointing into side 2.

Assume that the graphene sheet is located on a surface between two subdomains. Then, RTCs in (10) have to be modified to account for RBCs in (1) and (2). To derive these RRTC, first, RBCs (1) and (2) are rewritten as

$$\mathbf{M}_1 + \mathbf{M}_2 = 0 \quad (11)$$

$$\mathbf{J}_1 + \mathbf{J}_2 - \overline{\sigma}_g \cdot (\hat{\mathbf{n}}_1 \times \mathbf{M}_1) = 0 \quad (12)$$

$$\mathbf{J}_1 + \mathbf{J}_2 - \overline{\sigma}_g \cdot (\hat{\mathbf{n}}_2 \times \mathbf{M}_2) = 0. \quad (13)$$

Then, linearly combining (11) and (12) as (12) $- \hat{\mathbf{n}}_1 \times$ (11) and $\hat{\mathbf{n}}_1 \times$ (12) + (11) and using $\hat{\mathbf{n}}_1 = -\hat{\mathbf{n}}_2$ for \mathbf{J}_2 and \mathbf{M}_2 yield

$$\begin{aligned} \mathbf{J}_1 - \hat{\mathbf{n}}_1 \times \mathbf{M}_1 - \overline{\sigma}_g \cdot (\hat{\mathbf{n}}_1 \times \mathbf{M}_1) + \mathbf{J}_2 + \hat{\mathbf{n}}_2 \times \mathbf{M}_2 &= 0 \\ \hat{\mathbf{n}}_1 \times \mathbf{J}_1 + \mathbf{M}_1 + \overline{\sigma}_g \cdot \mathbf{M}_1 - \hat{\mathbf{n}}_2 \times \mathbf{J}_2 + \mathbf{M}_2 &= 0. \end{aligned} \quad (14)$$

This set of RRTC is used when \mathbf{r} approaches the surface from side 1. Linearly combining (11) and (13) as (13) $- \hat{\mathbf{n}}_2 \times$ (11) and $\hat{\mathbf{n}}_2 \times$ (13) + (11) and using $\hat{\mathbf{n}}_2 = -\hat{\mathbf{n}}_1$ for \mathbf{J}_1 and \mathbf{M}_1 yield

$$\begin{aligned} \mathbf{J}_2 - \hat{\mathbf{n}}_2 \times \mathbf{M}_2 - \overline{\sigma}_g \cdot (\hat{\mathbf{n}}_2 \times \mathbf{M}_2) + \mathbf{J}_1 + \hat{\mathbf{n}}_1 \times \mathbf{M}_1 &= 0 \\ \hat{\mathbf{n}}_2 \times \mathbf{J}_2 + \mathbf{M}_2 + \overline{\sigma}_g \cdot \mathbf{M}_2 - \hat{\mathbf{n}}_1 \times \mathbf{J}_1 + \mathbf{M}_1 &= 0. \end{aligned} \quad (15)$$

This set of RRTC is used when \mathbf{r} approaches the surface from side 2. As expected, (14) and (15) are the same except that variables with subscripts 1 and 2 are interchanged. Also, note that (11)–(13) can be recovered by adding (14) to (15) and subtracting (14) from (15),

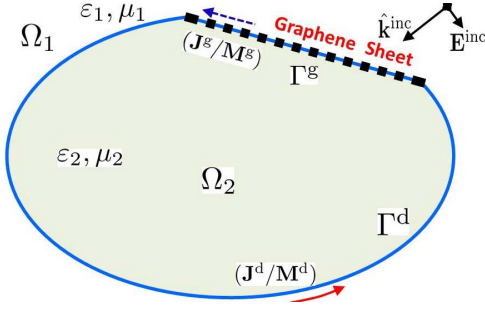


Fig. 1. Electromagnetic scattering from a graphene-based device.

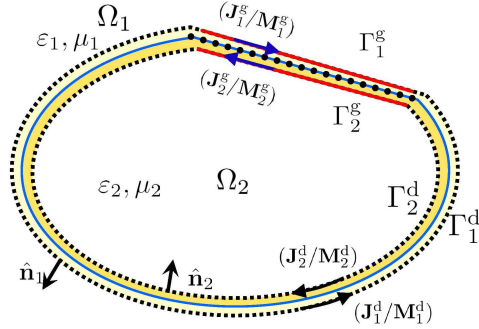


Fig. 2. Subdomains of the graphene-based device.

which also demonstrates that (14) and (15) are equivalent to (1) and (2) and they can be used to enforce these RBCs in the MT-SIE solver that is described in Section II-B.

B. MT-SIE Solver

The electromagnetic scattering scenario involving a graphene-based device is illustrated in Fig. 1. In this figure, Ω_1 and Ω_2 represent the dielectric substrate and the background medium, respectively. The graphene sheet is represented by Γ^g and is assumed to be located on the surface of the dielectric substrate. The part of the substrate surface, which is directly in touch with Ω_1 is represented by Γ^d . The permittivity, the permeability, the intrinsic impedance, and the wavenumber in Ω_m , $m \in \{1, 2\}$ are ϵ_m , μ_m , η_m , and k_m , respectively. The incident electromagnetic field, which originates in Ω_1 , is represented by $\{\mathbf{E}_1^{\text{inc}}, \mathbf{H}_1^{\text{inc}}\}$.

The computation domain is naturally decomposed into two nonoverlapping subdomains as shown in Fig. 2: the exterior subdomain Ω_1 with boundary $\partial\Omega_1$ and the inward-pointing unit normal vector $\hat{\mathbf{n}}_1$, and the interior dielectric subdomain Ω_2 with boundary $\partial\Omega_2$ and the inward-pointing unit outward normal vector $\hat{\mathbf{n}}_2$. The surfaces that represent the graphene sheet and the dielectric substrate Γ^g and Γ^d have two sides/faces, each of which ‘‘touches’’ Ω_1 and Ω_2 , that is, $\partial\Omega_m = \Gamma_m^g \cup \Gamma_m^d$, $m \in \{1, 2\}$.

In each subdomain Ω_m , a boundary value problem (BVP) with Maxwell equations can be setup. This BVP is same as the one in [30], [32], and [33], but differently, RBCs have to be enforced on the graphene surface. The full set of boundary conditions enforced on $\partial\Omega_m$ are expressed as

$$\pi_m^\times(\mathbf{H}_m) - \bar{\sigma}_g \cdot \pi_m^\tau(\mathbf{E}_m) = -\pi_n^\times(\mathbf{H}_n) \text{ on } \Gamma_m^g \quad (16)$$

$$\pi_m^\tau(\mathbf{E}_m) = \pi_n^\tau(\mathbf{E}_n) \text{ on } \partial\Omega_m = \Gamma_m^g \cup \Gamma_m^d \quad (17)$$

$$\pi_m^\times\left(\frac{1}{\mu_m}\nabla \times \mathbf{E}_m\right) = \pi_n^\times\left(\frac{1}{\mu_n}\nabla \times \mathbf{E}_n\right) \text{ on } n \Gamma_m^d \quad (18)$$

where $m, n \in \{1, 2\}$, $m \neq n$, $\{\mathbf{E}_m, \mathbf{H}_m\}$ are the electromagnetic fields in Ω_m , and the trace operators $\pi_m^\tau(\mathbf{u}) = \hat{\mathbf{n}}_m \times (\mathbf{u} \times \hat{\mathbf{n}}_m)|_{\partial\Omega_m}$ and $\pi_m^\times(\mathbf{u}) = \hat{\mathbf{n}}_m \times \mathbf{u}|_{\partial\Omega_m}$ represent tangential and twisted tangential components of \mathbf{u} on $\partial\Omega_m$, respectively. Electromagnetic fields in Ω_m satisfy the fundamental field relations $\mathbf{E}_m = \mathbf{E}_m^{\text{sca}} + \mathbf{E}_m^{\text{inc}}$ and $\mathbf{H}_m = \mathbf{H}_m^{\text{sca}} + \mathbf{H}_m^{\text{inc}}$. Note that $\mathbf{E}_2^{\text{inc}}$ and $\mathbf{H}_2^{\text{inc}}$ are zero for the scattering problem considered here. Using Stratton-Chu representation, the scattered fields $\mathbf{E}_m^{\text{sca}}$ and $\mathbf{H}_m^{\text{sca}}$, $m \in \{1, 2\}$, are expressed as [40]

$$\begin{aligned} \mathbf{E}_m^{\text{sca}} &= \eta_m \mathcal{L}_m\{\mathbf{J}_m^d\} - \eta_0 \mathcal{K}_m\{\mathbf{M}_m^d\} + \eta_m \mathcal{L}_m\{\mathbf{J}_m^g\} \\ &\quad - \eta_0 \mathcal{K}_m\{\mathbf{M}_m^g\} \\ \eta_m \mathbf{H}_m^{\text{sca}} &= \eta_m \mathcal{K}_m\{\mathbf{J}_m^d\} + \eta_0 \mathcal{L}_m\{\mathbf{M}_m^d\} + \eta_m \mathcal{K}_m\{\mathbf{J}_m^g\} \\ &\quad + \eta_0 \mathcal{L}_m\{\mathbf{M}_m^g\} \end{aligned} \quad (19)$$

where η_0 is the intrinsic impedance in free space, $\mathbf{J}_m^d = \hat{\mathbf{n}}_m \times \mathbf{H}_{\Gamma_m^d}$ and $\mathbf{M}_m^d = -\hat{\mathbf{n}}_m \times \mathbf{E}_{\Gamma_m^d}$ and $\mathbf{J}_m^g = \hat{\mathbf{n}}_m \times \mathbf{H}_{\Gamma_m^g}$ and $\mathbf{M}_m^g = -\hat{\mathbf{n}}_m \times \mathbf{E}_{\Gamma_m^g}$ are the (unknown) equivalent electric and magnetic currents introduced on Γ_m^d and Γ_m^g , respectively. In (19), operators \mathcal{L}_m and \mathcal{K}_m are given by Zhao *et al.* [32], [33]

$$\begin{aligned} \mathcal{L}_m\{\mathbf{X}_m^e\}(\mathbf{r}) &= -jk_m \int_{\Gamma_m^e} \left[\mathbf{I} + \frac{1}{k_m^2} \nabla \nabla \cdot \right] \mathbf{X}_m^e(\mathbf{r}') G_m(\mathbf{r}, \mathbf{r}') ds' \\ \mathcal{K}_m\{\mathbf{X}_m^e\}(\mathbf{r}) &= \int_{\Gamma_m^e} \nabla G_m(\mathbf{r}, \mathbf{r}') \times \mathbf{X}_m^e(\mathbf{r}') ds' \end{aligned}$$

where $e \in \{d, g\}$ and G_m is the Green function of the unbounded medium with wavenumber k_m . Note that $\mathcal{K}_m\{\mathbf{X}_m^e\} = \hat{\mathbf{n}}_m \times \mathbf{X}_m^e/2 + \bar{\mathcal{K}}_m\{\mathbf{X}_m^e\}$, where $\bar{\mathcal{K}}_m$ is the principal value of \mathcal{K}_m . Inserting (19) into the tangential components of the fundamental field relations on Γ_m^d and Γ_m^g yield \mathbf{E} - and \mathbf{H} -field equations in Ω_m as [28]

$$\begin{aligned} \frac{\eta_0}{2} \pi_m^\times(\mathbf{M}_m^d) + \eta_0 \pi_m^\tau(\bar{\mathcal{K}}_m\{\mathbf{M}_m^d\} + \mathcal{K}_m\{\mathbf{M}_m^g\}) \\ - \eta_m \pi_m^\tau(\mathcal{L}_m\{\mathbf{J}_m^d\} + \mathcal{L}_m\{\mathbf{J}_m^g\}) &= \pi_m^\tau(\mathbf{E}_m^{\text{inc}}) \text{ on } \Gamma_m^d \\ - \frac{\eta_0}{2} \pi_m^\times(\mathbf{J}_m^d) - \eta_0 \pi_m^\tau(\mathcal{K}_m\{\mathbf{J}_m^d\} + \bar{\mathcal{K}}_m\{\mathbf{J}_m^g\}) \\ - \frac{\eta_0}{\eta_m} \pi_m^\tau(\mathcal{L}_m\{\mathbf{M}_m^d\} + \mathcal{L}_m\{\mathbf{M}_m^g\}) &= \eta_0 \pi_m^\tau(\mathbf{H}_m^{\text{inc}}) \text{ on } \Gamma_m^d \quad (20) \\ \frac{\eta_0}{2} \pi_m^\times(\mathbf{M}_m^g) + \eta_0 \pi_m^\tau(\mathcal{K}_m\{\mathbf{M}_m^d\} + \bar{\mathcal{K}}_m\{\mathbf{M}_m^g\}) \\ - \eta_m \pi_m^\tau(\mathcal{L}_m\{\mathbf{J}_m^d\} + \mathcal{L}_m\{\mathbf{J}_m^g\}) &= \pi_m^\tau(\mathbf{E}_m^{\text{inc}}) \text{ on } \Gamma_m^g \\ - \frac{\eta_0}{2} \pi_m^\times(\mathbf{J}_m^g) - \eta_0 \pi_m^\tau(\mathcal{K}_m\{\mathbf{J}_m^d\} + \bar{\mathcal{K}}_m\{\mathbf{J}_m^g\}) \\ - \frac{\eta_0}{\eta_m} \pi_m^\tau(\mathcal{L}_m\{\mathbf{M}_m^d\} + \mathcal{L}_m\{\mathbf{M}_m^g\}) &= \eta_0 \pi_m^\tau(\mathbf{H}_m^{\text{inc}}) \text{ on } \Gamma_m^g. \quad (21) \end{aligned}$$

To enforce the boundary conditions (16)–(18), (20) and (10) are combined on Γ_m^d and (21) and (14) are combined on Γ_m^g , leading to

$$\begin{aligned} \frac{\eta_0}{2} \mathbf{J}_m^d - \eta_0 \eta_m \pi_m^\tau(\mathcal{L}_m\{\mathbf{J}_m^d\} + \mathcal{L}_m\{\mathbf{J}_m^g\}) \\ - \eta_0 \pi_m^\tau(\bar{\mathcal{K}}_m\{\mathbf{M}_m^d\} + \mathcal{K}_m\{\mathbf{M}_m^g\}) \\ + \frac{\eta_0}{2} \mathbf{J}_n^d + \frac{\eta_0}{2} \pi_n^\times(\mathbf{M}_n^d) &= \pi_m^\tau(\mathbf{E}_m^{\text{inc}}) \text{ on } \Gamma_m^d \\ \frac{\eta_0}{2} \mathbf{M}_m^d - \frac{\eta_0}{\eta_m} \pi_m^\tau(\mathcal{L}_m\{\mathbf{M}_m^d\} + \mathcal{L}_m\{\mathbf{M}_m^g\}) \\ - \eta_0 \pi_m^\tau(\bar{\mathcal{K}}_m\{\mathbf{J}_m^d\} + \mathcal{K}_m\{\mathbf{J}_m^g\}) \\ + \frac{\eta_0}{2} \mathbf{M}_n^d - \frac{\eta_0}{2} \pi_n^\times(\mathbf{J}_n^d) &= \eta_0 \pi_m^\tau(\mathbf{H}_m^{\text{inc}}) \text{ on } \Gamma_m^d \quad (22) \\ \frac{\eta_0}{2} \mathbf{J}_m^g - \frac{\eta_0}{2} \bar{\sigma}_g \cdot \pi_m^\times(\mathbf{M}_m^g) - \eta_0 \eta_m \pi_m^\tau(\mathcal{L}_m\{\mathbf{J}_m^d\} + \mathcal{L}_m\{\mathbf{J}_m^g\}) \\ + \eta_0 \pi_m^\tau(\mathcal{K}_m\{\mathbf{M}_m^d\} + \bar{\mathcal{K}}_m\{\mathbf{M}_m^g\}) \\ + \frac{\eta_0}{2} \mathbf{J}_n^g + \frac{\eta_0}{2} \pi_n^\times(\mathbf{M}_n^g) &= \pi_m^\tau(\mathbf{E}_m^{\text{inc}}) \text{ on } \Gamma_m^g \\ \frac{\eta_0}{2} \mathbf{M}_m^g + \frac{\eta_0}{2} \bar{\sigma}_g \cdot \mathbf{M}_m^g - \frac{\eta_0}{\eta_m} \pi_m^\tau(\mathcal{L}_m\{\mathbf{M}_m^d\}) \end{aligned}$$

$$\begin{aligned}
 & + \mathcal{L}_m\{\mathbf{M}_m^g\} - \eta_0\pi_m^\tau(\mathcal{K}_m\{\mathbf{J}_m^d\} + \overline{\mathcal{K}}_m\{\mathbf{J}_m^g\}) \\
 & + \frac{\eta_0}{2}\mathbf{M}_n^g - \frac{\eta_0}{2}\pi_n^\times(\mathbf{J}_n^g) = \eta_0\pi_m^\tau(\mathbf{H}^{\text{inc}}) \text{ on } \Gamma_m^g. \quad (23)
 \end{aligned}$$

To numerically solve (22) and (23), first Γ^d and Γ^g are discretized into a mesh of triangular patches. Then, the unknown electric and magnetic currents on Γ_m^d and Γ_m^g , $m \in \{1, 2\}$, are expanded using RWG basis function sets \mathbf{j}_m and \mathbf{m}_m , respectively [29]. Inserting these expansions into (22) and (23) and applying the Galerkin testing to the resulting equations yield a linear matrix system

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{M}_{12} \\ \mathbf{M}_{21} & \mathbf{A}_2 \end{bmatrix} \begin{bmatrix} \mathbf{I}_1 \\ \mathbf{I}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{V}_0 \\ \mathbf{0} \end{bmatrix} \quad (24)$$

where matrices \mathbf{A}_m and \mathbf{M}_{mn} , $m, n \in \{1, 2\}$, $n \neq m$, represent the ‘‘self’’ and ‘‘coupled’’ electromagnetic interactions in Ω_m and between Ω_m and Ω_n , respectively. Vectors \mathbf{I}_m store the unknown coefficients of basis function sets \mathbf{j}_m and \mathbf{m}_m and \mathbf{V}_0 stores the tested incident fields. \mathbf{A}_m are dense matrices and expressed as

$$\mathbf{A}_m = \begin{bmatrix} \mathbf{A}_m^{\text{JJ}} & \mathbf{A}_m^{\text{JM}} \\ \mathbf{A}_m^{\text{MJ}} & \mathbf{A}_m^{\text{MM}} \end{bmatrix} \quad (25)$$

where the each matrix block is given by

$$\begin{aligned}
 \mathbf{A}_m^{\text{JJ}} &= \left\langle \mathbf{j}_m, \frac{\eta_0}{2}\mathbf{j}_m - \eta_n\pi_m^\tau(\mathcal{L}_m\{\mathbf{j}_m\}) \right\rangle_{\partial\Omega_m} \\
 \mathbf{A}_m^{\text{JM}} &= \left\langle \mathbf{j}_m, \eta_0\pi_m^\tau(\overline{\mathcal{K}}_m\{\mathbf{m}_m\}) \right\rangle_{\partial\Omega_m} \\
 & \quad - \left\langle \mathbf{j}_m, \frac{\eta_0}{2}\overline{\sigma}_g \cdot \pi_m^\times(\mathbf{m}_m) \right\rangle_{\Gamma_m^g} \\
 \mathbf{A}_m^{\text{MJ}} &= \left\langle \mathbf{m}_m, -\eta_0\pi_m^\tau(\overline{\mathcal{K}}_m\{\mathbf{j}_m\}) \right\rangle_{\partial\Omega_m} \\
 \mathbf{A}_m^{\text{MM}} &= \left\langle \mathbf{m}_m, \frac{\eta_0}{2}\mathbf{m}_m - \frac{1}{\eta_m}\pi_m^\tau(\mathcal{L}_m\{\mathbf{m}_m\}) \right\rangle_{\partial\Omega_m} \\
 & \quad + \left\langle \mathbf{m}_m, \frac{\eta_0}{2}\overline{\sigma}_g \cdot \mathbf{m}_m \right\rangle_{\Gamma_m^g}. \quad (26)
 \end{aligned}$$

Here, $\langle \mathbf{u}, \mathbf{v} \rangle$ denotes the inner product of two complex vector functions \mathbf{u} and \mathbf{v}

$$\langle \mathbf{u}, \mathbf{v} \rangle_\Gamma = \int_\Gamma (\mathbf{u} \cdot \mathbf{v}) d\Gamma. \quad (27)$$

Since the coupling between electromagnetic fields in two subdomains is accounted for using RTCs and RRTC, matrices \mathbf{M}_{mn} are sparse. They are expressed as

$$\mathbf{M}_{mn} = \begin{bmatrix} \frac{\eta_m}{2} \langle \mathbf{j}_m, \mathbf{j}_n \rangle_{\partial\Omega_m} & \frac{\eta_0}{2} \langle \mathbf{j}_m, \pi_n^\times(\mathbf{m}_n) \rangle_{\partial\Omega_m} \\ \frac{\eta_0}{2} \langle \mathbf{m}_m, \pi_n^\times(\mathbf{j}_n) \rangle_{\partial\Omega_m} & -\frac{\eta_m}{2} \langle \mathbf{m}_m, \mathbf{m}_n \rangle_{\partial\Omega_m} \end{bmatrix}. \quad (28)$$

In (25), the right-hand side vector $\mathbf{V}_0 = [\mathbf{V}_0^J \mathbf{V}_0^M]^T$, where

$$\begin{aligned}
 \mathbf{V}_0^J &= \left\langle \mathbf{j}_0, \pi_m^\tau(\mathbf{E}^{\text{inc}}) \right\rangle_{\partial\Omega_0} \\
 \mathbf{V}_0^M &= \left\langle \mathbf{m}_0, \eta_0\pi_m^\tau(\mathbf{H}^{\text{inc}}) \right\rangle_{\partial\Omega_0}. \quad (29)
 \end{aligned}$$

The matrix system (24) is solved iteratively using the generalized minimal residual method scheme (GMRES) [41]. The computational cost of multiplying \mathbf{A}_1 and \mathbf{A}_2 by vectors scales as $O(N^2)$. While using the multilevel fast multipole algorithm (MLFMA), the cost is reduced to $O(N \log N)$ [42], [43]. The computational cost of multiplying sparse matrices \mathbf{M}_{12} and \mathbf{M}_{21} by vectors is $O(N)$.

III. NUMERICAL RESULTS

In this section, several numerical examples, which demonstrate the accuracy and the applicability of the proposed MT-SIE solver, are presented. In all examples, it is assumed that the background medium Ω_1 is free space with permittivity ϵ_0 and permeability μ_0 , and the

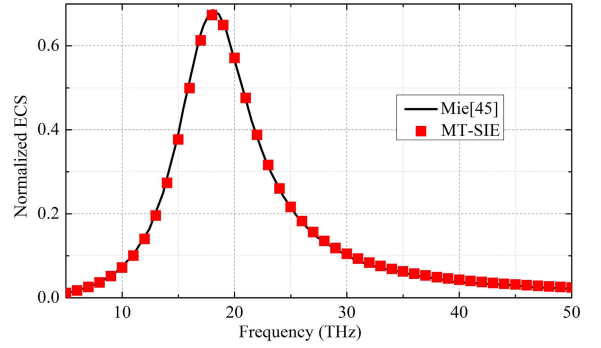


Fig. 3. Normalized ECS of the spherical graphene surface.

excitation is a plane wave with electric field $\mathbf{E}^{\text{inc}}(\mathbf{r}) = E_0 \hat{\mathbf{p}} e^{-jk_0 \hat{\mathbf{k}} \cdot \mathbf{r}}$. Here, $E_0 = 1$ V/m is the amplitude, $\hat{\mathbf{p}}$ is the polarization vector, $\hat{\mathbf{k}}$ is the direction of propagation, and $k_0 = 2\pi/\lambda_0$ and λ_0 are the wavenumber and the wavelength in free space, respectively. The substrates are nonmagnetic with permeability μ_0 . For all examples considered in this section, the GMRES iterations are terminated when the relative residual reaches 0.001.

A. Nonmagnetized Spherical Graphene Surface

In the first example, scattering from a spherical graphene surface is investigated. The surface is centered at the origin, its radius is 200 nm, and the permittivity and the permeability inside the surface are ϵ_0 and μ_0 , respectively. The parameters of the graphene are $\mu_c = 0.3$ eV and $\tau = 0.02$ ps. The excitation parameters are $\hat{\mathbf{p}} = \hat{\mathbf{x}}$ and $\hat{\mathbf{k}} = -\hat{\mathbf{z}}$, and the frequency is swept from 0.5 to 50 THz. The spherical surface is discretized using 532 triangular patches, which corresponds to an average edge length of 45 nm ($\lambda_0/133$ at 50 THz).

First, the equivalent electric and magnetic currents on the inner and outer surfaces of the sphere are computed by solving (24). Then, the currents on the outer surface are used to compute the extinction cross section (ECS) [44], [45]. Fig. 3 compares this ECS (which is normalized by the sphere’s geometrical cross section) to ECS computed using the analytical solution [46]. The results agree very well, which demonstrates the accuracy of the proposed MT-SIE solver.

B. Magnetized Graphene Patch

In this example, scattering from a magnetized graphene patch of dimensions $10 \mu\text{m} \times 2 \mu\text{m}$ (along x - and y -directions, respectively) is investigated. It is assumed that the patch is centered on the top surface of a substrate with dimensions $10 \mu\text{m} \times 2 \mu\text{m} \times 0.15 \mu\text{m}$ (along x -, y -, and z -directions, respectively). The permittivity of the substrate is ϵ_0 . This ensures that the structure simulated by the MT-SIE solver is equivalent to a magnetized graphene patch that resides in free space. The parameters of the graphene are $\tau = 0.33$ ps, $B_0 = 0.25$ T, and $\mu_c \in \{0.5, 1.0, 1.5\}$ eV. The excitation parameters are $\hat{\mathbf{p}} = \hat{\mathbf{x}}$ and $\hat{\mathbf{k}} = -\hat{\mathbf{z}}$, and the frequency is swept from 0.1 to 10 THz. The surfaces of the patch and the substrate are discretized into 474 and 632 triangular patches, respectively, which corresponds to an average edge length of $0.3 \mu\text{m}$ ($\lambda_0/100$ at 10 THz).

Fig. 4 plots the absorption cross section (ACS) [44], [45] obtained using the equivalent currents computed by the MT-SIE solver for three different values of μ_c and compares it to ACS provided in [19] and [21]. Results agree well.

C. Magnetized Graphene Patch on a Dielectric Substrate

Next, scattering from a magnetized graphene patch of dimensions $150 \mu\text{m} \times 150 \mu\text{m}$ (along x - and y -directions, respectively), which

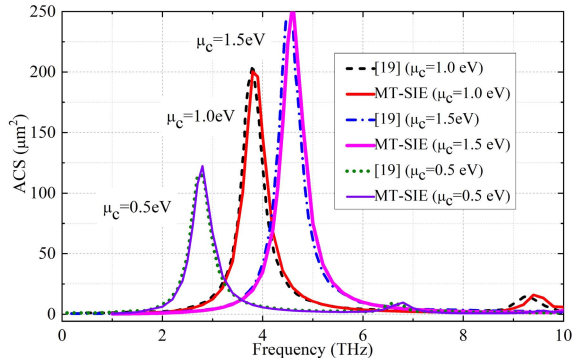


Fig. 4. ACS of the magnetized graphene sheet for $\mu_c \in \{0.5, 1.0, 1.5\}$ eV.

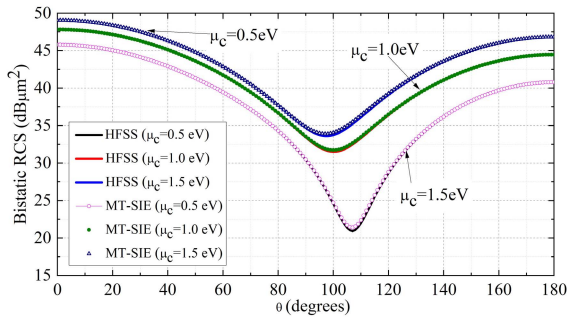


Fig. 5. Bistatic RCS of the magnetized graphene sheet on a dielectric substrate for $\mu_c \in \{0.5, 1.0, 1.5\}$ eV.

is centered on the top surface of a dielectric substrate of dimensions $150 \mu\text{m} \times 150 \mu\text{m} \times 30 \mu\text{m}$ (along x -, y -, and z -directions, respectively) is investigated. The permittivity of the substrate is $4.0\epsilon_0$. The parameters of the graphene and the excitation are the same as those in the previous example. The frequency is 1 THz. The surfaces of the patch and the substrate are discretized into 208 and 584 triangular patches, respectively, which corresponds to an average edge length of $15 \mu\text{m}$ ($\lambda_0/20$ at 1 THz).

Fig. 5 plots the copolarized bistatic radar cross section (RCS) (on the $\phi = 0$ plane) obtained using the equivalent currents computed by the MT-SIE solver for $\mu_c \in \{0.5, 1.0, 1.5\}$ eV and compares it to RCS obtained using the finite-element method-based commercial software HFSS. Results agree well and also show that RCS decreases with increasing μ_c . For this example, GMRES (without a preconditioner) requires 153, 175, and 189 iterations for simulations with $\mu_c = 0.5, 1.0,$ and 1.5 eV, respectively.

D. THz Polarization Converter

In this example, scattering from a tunable THz reflective linear polarization converter is analyzed [47]. The geometry and the dimensions of the structure are shown in Fig. 6. The permittivity of the substrate is $2.2\epsilon_0$. The parameters of the graphene are $\mu_c = 0.5$ eV and $\tau = 1.0$ ps and the excitation parameters are $\hat{\mathbf{p}} = \hat{\mathbf{x}}$ and $\hat{\mathbf{k}} = -\hat{\mathbf{z}}$. The frequency is 1 THz. The surfaces of the 49 oval-shaped patches and the substrate are discretized using 3871 and 3709 triangular patches, respectively, which corresponds to an average edge length of $13 \mu\text{m}$ ($\lambda_0/25$ at 1 THz).

Fig. 7 plots the copolarized and cross-polarized bistatic RCS (on $\phi = 0$ plane) obtained using the equivalent currents computed by the MT-SIE solver and compares it to RCS obtained using HFSS. Results agree well. The figure also shows that the cross-polarized reflection is enhanced by the polarization converter. Table I compares the computational requirements of the MT-SIE solver (without a preconditioner

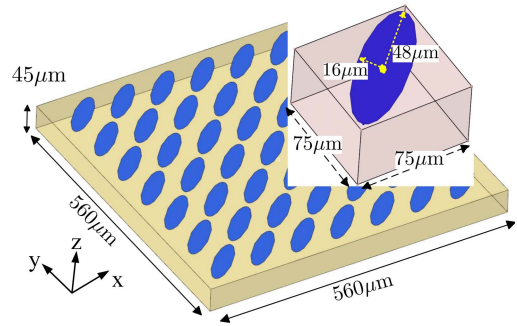


Fig. 6. Geometry and the dimensions of the THz polarization converter.

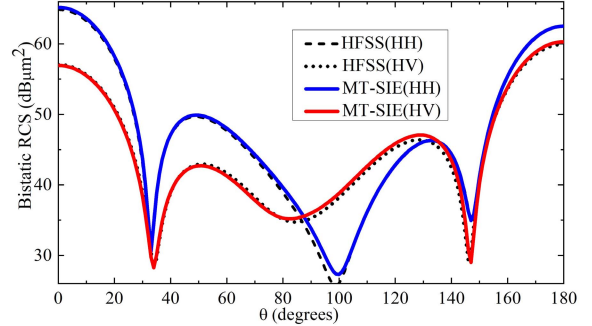


Fig. 7. Copolarized and cross-polarized RCS of the THz polarization converter.

TABLE I
COMPUTATIONAL REQUIREMENTS FOR SIMULATIONS
OF THE THz POLARIZATION CONVERTER

	Time	Memory	Iterations
MT-SIE (SAI preconditioner)	30 m	2.99 GB	30
MT-SIE (no preconditioner)	10 m	1.58 GB	399
HFSS	1 h 54 m	42.1 GB	N/A

and with the sparse-approximate-inverse (SAI) preconditioner [48]) to those of HFSS and clearly shows that the MT-SIE solver is faster and uses significantly less memory.

IV. CONCLUSION

An MT-SIE solver is formulated and implemented to analyze electromagnetic field interactions on composite devices involving graphene sheets. This solver decomposes the computation domain into exterior and interior subdomains, which represent the unbounded background medium and the dielectric substrate, respectively. The electric and magnetic field equations are used as the governing equations in each subdomain. RRTCs are derived for the first time to account for the infinitesimally thin graphene sheet that is located on the interface between these two subdomains. The governing equations of a subdomain are locally coupled to the governing equations of its neighbor using RRTCs and RTCs. The accuracy and the applicability of the MT-SIE solver are demonstrated by various numerical examples.

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