Modified Combined Tangential Formulation for Stable and Accurate Analysis of Plasmonic Structures

Barışcan Karaosmanoğlu and Özgür Ergül

Department of Electrical and Electronics Engineering
Middle East Technical University, Ankara, Turkey
{bariscan,ozergul}@metu.edu.tr

Abstract ─ We consider a modified combined tangential formulation (MCTF) for stable and accurate analysis of plasmonic problems involving metallic objects modeled as penetrable bodies. For a wide range of negative real permittivity values, corresponding to varying characteristics of metals at THz, infrared, and visible frequencies, MCTF provides accurate solutions in comparison to the conventional formulations for penetrable objects. We further show that, for structures with subwavelength dimensions, penetrable models formulated with MCTF can be essential for accurate analysis, rather than the perfectly conducting formulations, even at the lower THz frequencies.

Index Terms ─ Plasmonic problems, scattering, surface integral equations.

I. INTRODUCTION

Most metals at optical frequencies are known to possess plasmonic properties, which can be employed in diverse applications, such as sensing, energy harvesting, optical links, and super-resolution. In parallel with this, for numerical modeling of plasmonic structures involving arbitrary geometries, traditional solvers have been modified to handle negative permittivity values that can be used to represent metals at optical frequencies [1]. While volume formulations are mostly used in this area, plasmonic problems with increasing complexity and sizes often need more efficient solvers that are based on surface formulations [2]–[5]. In fact, if the structures can be represented as homogeneous or piecewise homogeneous objects, surface integral equations can provide the desired efficiency without sacrificing the accuracy. On the other hand, since most of the formulations have been developed for ordinary dielectric and magnetic objects [6], new numerical problems arise when the traditional solvers are employed to analyze plasmonic structures.

As a background of this study, we refer to [7] and [8], where we showed that the conventional formulations may require very dense discretizations with respect to wavelength in order to obtain sufficient accuracy for plasmonic objects, while some formulations even break down as the negative permittivity increases. Therefore, we need more accurate and stable formulations that can be used in wide ranges of permittivity values, especially for increasingly large negative permittivities to close the gap towards perfect electric conductor (PEC) models. We recently introduced a modified combined tangential formulation (MCTF) that falls into this category and we showed the advantages of MCTF over other penetrable formulations for plasmonic structures of several wavelengths [10]. Specifically, MCTF provides accurate and stable solutions for large permittivity values that are typical at the infrared and higher THz frequencies. In this contribution, we further show the advantages of MCTF at much lower frequencies. When the frequency drops to lower THz ranges, PEC models are assumed to be valid, while this is not true if the dimensions of the structures are very small with respect to wavelength. Therefore, penetrable formulations may still be needed, even when the frequency is low. As shown in this letter, MCTF can also provide accurate analysis of such subwavelength metallic objects, in comparison to the conventional PEC models and their typical formulations with the electric-field integral equation (EFIE).

II. MCTF FOR DIFFERENT REGIMES

MCTF is a tangential formulation, similar to the combined tangential formulation (CTF) and the variants of the Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation. Hence, with the low-order discretizations employing the Rao-Wilton-Glisson functions and Galerkin scheme, it naturally provides more accurate solutions than the normal and mixed formulations [9], such as the electric and magnetic current combined-field integral equation (JMCFIE). For plasmonic problems involving structures comparable to wavelength, the advantages of MCTF are its higher efficiency in comparison to PMCHWTs, its better stability in comparison to CTF, and its better accuracy in comparison to JMCFIE and similar normal/mixed formulations [10].

In the frequency domain, matrix equations derived

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from MCTF can be written as [10]:

$$\bar{\boldsymbol{Z}} = \begin{bmatrix} \eta_o \bar{\boldsymbol{T}}_o + \eta_p \bar{\boldsymbol{T}}_p & \left(-\bar{\boldsymbol{K}}_o - \bar{\boldsymbol{K}}_p\right) \\ \eta_o \eta_p \left(-\bar{\boldsymbol{K}}_o - \bar{\boldsymbol{K}}_p\right) & \eta_p \bar{\boldsymbol{T}}_o + \eta_o \bar{\boldsymbol{T}}_p \end{bmatrix}, \qquad (1)$$

where $\bar{\boldsymbol{T}}_{o,p}$ and $\bar{\boldsymbol{K}}_{o,p}$ are the electric-field integral operator and the magnetic-field integral operator, respectively, which are tested tangentially $(\hat{\boldsymbol{a}}_n \times \hat{\boldsymbol{a}}_n \times)$, i.e.,

$$\bar{\boldsymbol{T}}_u[m,n] = ik_u \left\langle \boldsymbol{t}_m(\boldsymbol{r}), g_u(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{b}_n(\boldsymbol{r}')\right\rangle - \frac{i}{k_u}\left\langle \boldsymbol{t}_m(\boldsymbol{r}), \nabla' \cdot \boldsymbol{b}_n(\boldsymbol{r}')\nabla' g_u(\boldsymbol{r},\boldsymbol{r}')\right\rangle, \qquad (2)$$

$$\bar{\boldsymbol{K}}_u[m,n] = \left\langle \boldsymbol{t}_m(\boldsymbol{r}), \boldsymbol{b}_n(\boldsymbol{r}') \times \nabla' g_u(\boldsymbol{r},\boldsymbol{r}')\right\rangle, \qquad (3)$$

for $u = o$ (outer/vacuum) and $u = p$ (inner/plasmonic). In the above, $\eta_u = \sqrt{\mu_u}/\sqrt{\varepsilon_u}$ represents the intrinsic impedance, $k_u = \omega\sqrt{\mu_u}\sqrt{\varepsilon_u} = 2\pi/\lambda_u$ represents the wavenumber, and $g_u(\boldsymbol{r},\boldsymbol{r}') = \exp(ik_u|\boldsymbol{r} - \boldsymbol{r}'|)/4\pi|\boldsymbol{r} - \boldsymbol{r}'|$ is the homogeneous-space Green's function. In addition, $\boldsymbol{t}_m$ and $\boldsymbol{b}_n$ represent testing and basis functions (the same set of the RWG functions). The limit term in the MFIE operator is extracted, as usual.

A. Fixed electrical size

Considering a metallic object with a fixed electrical size, i.e., *kD*=constant, increasing negative permittivity $(\varepsilon_R \to -\infty)$ leads to $(\eta_p \to 0)$, $(k_p \to i\infty)$, and,

$$\lim_{\varepsilon_R \to -\infty} \bar{\boldsymbol{T}}_p = -\bar{\boldsymbol{I}}/2, \qquad \lim_{\varepsilon_R \to -\infty} \bar{\boldsymbol{K}}_p = 0, \qquad (4)$$

where $\bar{\boldsymbol{I}} = \left\langle \boldsymbol{t}_m(\boldsymbol{r}), \boldsymbol{b}_n(\boldsymbol{r}')\right\rangle$. Then, MCTF turns into EFIE as:

$$\lim_{\varepsilon_R \to -\infty} \bar{\boldsymbol{Z}} = \eta_o \begin{bmatrix} \bar{\boldsymbol{T}}_o & -\bar{\boldsymbol{K}}_o \\ 0 & -\bar{\boldsymbol{I}}/2 \end{bmatrix}, \qquad (5)$$

where the second row makes the magnetic current zero (due to vanishing small right-hand side of this row). With a well balance of the matrix blocks [10], convergence to EFIE is achieved via a vanishing $\eta_p \bar{\boldsymbol{T}}_p$, hence without a numerical problem. We note that all penetrable formulations should reduce into an appropriate PEC form; however, this can be numerically difficult for many conventional formulations. The limiting process is useful to show the stability of MCTF as the frequency goes down for a fixed electrical size and the object becomes PEC.

B. Fixed metric size

For an object with a fixed metric size, decreasing frequency has a different effect, since the material tends to become perfectly conducting, but at the same time, the object becomes electrically small. In fact, there is a balance between material and size, i.e., $\omega \to 0$, $\varepsilon_R \to -\infty$, $\eta_p \to 0$, $k_p \sim$ constant, and,

$$\eta_p \bar{\boldsymbol{T}}_p \sim c\left\langle \boldsymbol{t}_m(\boldsymbol{r}), \nabla' \cdot \boldsymbol{b}_n(\boldsymbol{r}')\nabla' g_u(\boldsymbol{r},\boldsymbol{r}')\right\rangle, \qquad (6)$$

The constant c in (6) depends on the type of the metal and the model used (Drude, Lorentz-Drude, etc.). But, the bottomline is that MCTF in (5) does not converge into a PEC formulation. In fact, localization of the inner interactions as the negative permittivity increases is balanced with the decreasing electrical size of the object. Therefore, MCTF provides more correct interpretation of the physical problem, while using a PEC model and a related integral equation may lead to deviating results, as shown below.

III. NUMERICAL RESULTS

First, we consider the stability and accuracy of MCTF for a fixed electrical size. Fig. 1 presents the results of scattering problems involving plasmonic spheres of diameter $1.04\lambda_O$. For the relative permittivity, we consider different values $\varepsilon_r = (\varepsilon_R + i)$, where ε_R changes from –512 to 32. The spheres are illuminated by plane waves. For numerical solutions, the problems are discretized with $\lambda_O/10$ triangles, leading to matrix equations involving 2166 unknowns. In addition to different formulations, the problems are solved via Mie series to obtain reference values. In Fig. 1, the relative error in the far-zone electric field and the number of GMRES iterations (for 10^{-4} residual error, without preconditioning and restart) are plotted with respect to ε_R. For positive values of ε_R, it can be observed that the accuracy deteriorates as the contrast increases, as a result of increasing geometric deviation, integration problems, formulation issues (unbalanced blocks, ill conditioning, etc.), or the combination of these problems. Focusing on the negative values, we observe that JMCFIE results have very large errors that become relatively smaller, but still significant, as the contrast increases. In the same direction (increasing contrast), the error of CTF increases dramatically up to around 20% when $\varepsilon_R = -512$. Interestingly, the number of iterations for CTF drops, showing that the increasing error is not related to conditioning. MCTF has the same accuracy as PMCHWT and its scaled (balanced) version PMCHWT-S. All these these formulations provide quite stable results in terms of the accuracy for all negative values of ε_R. On the other hand, MCTF requires less iterations than PMCHWT (especially for small values of negative ε_R) and PMCHWT-S (especially for large values of negative ε_R). Hence, in terms of the efficiency, MCTF is more reliable than PMCWHTs for plasmonic simulations.

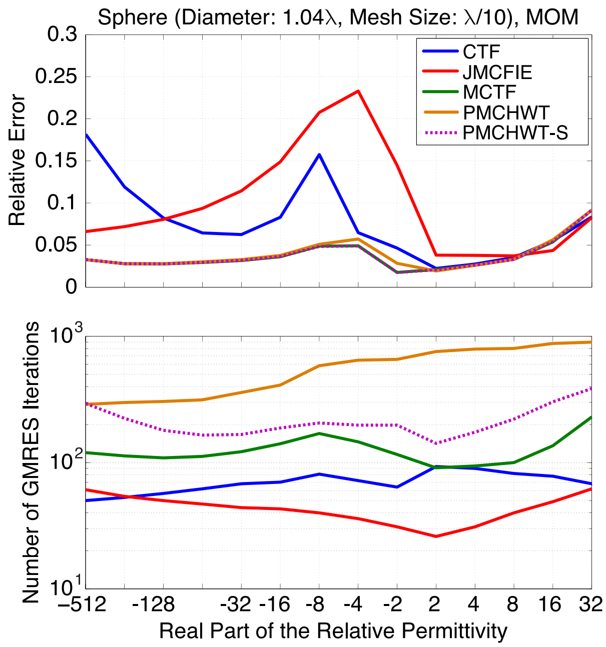

Fig. 1. Solutions of scattering problems involving spheres of diameter $1.04\lambda_O$. Far-zone relative errors and iteration counts are investigated with respect to the relative real permittivity values.

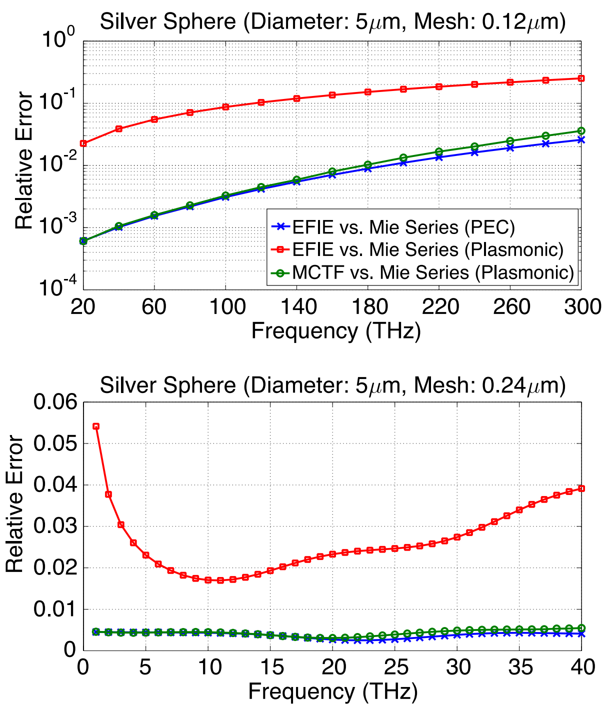

Fig. 2. Solutions of scattering problems involving a silver sphere of diameter $5\ \mu m$. Far-zone relative errors in numerical solutions are investigated with respect to the frequency. Reference solutions are obtained by using Mie-series for plasmonic (silver) and PEC cases.

Next, we consider the stability and accuracy of MCTF for a fixed metric size. Figure 2 presents the results of scattering problems involving a silver sphere of diameter $5\ \mu m$ illuminated by plane waves. The Lorentz-Drude model is used for the relative permittivity of the silver. In Fig. 2, the relative errors (in the far-zone electric field) in the numerical solutions of MCTF and EFIE (PEC model) in comparison to the plasmonic Mie-series solutions are plotted. In the 20–300 THz range (discretization size $0.12\ \mu m$), where the sphere size is approximately $0.33-5\lambda_O$, the error in the EFIE solutions decreases down to 2% as the frequency drops. However, as shown in the plot for the 0–40 THz range, the EFIE error increases back to 5% when the frequency further drops. The error in MCTF with respect to plasmonic Mie-series solutions is mostly below 1% (larger errors occurs above 180 THz since the discretization size with respect to wavelength is large), while it is completely stable in the 0–40 THz range. Finally, as also shown in Fig. 2, EFIE is consistent with the PEC Mie-series solutions, indicating that the perfectly conducting model itself deviates from the physical (silver) model, despite the frequency drops down to several THz.

IV. CONCLUSION

We present the accuracy and stability of MCTF for plasmonic problems involving metallic objects with negative permittivity values. Considering objects comparable to the wavelength, MCTF provides accurate solutions for different permittivity values, leading to stable plasmonic-to-PEC transition as the negative permittivity gets larger. We further show that, small objects with respect to wavelength may also require penetrable models (hence, MCTF) despite the frequency can be only in the order of several THz. These results on canonical objects make MCTF attractive for the analysis of metallic structures with different sizes at THz, infrared, and higher optical frequencies.

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Barışcan Karaosmanoğlu received the B.Sc. degree in Electronics and Communication Engineering from Doğuş University, Istanbul, Turkey, in 2011, and the M.S. degree in Electrical and Electronics Engineering from Bilkent University, Ankara, Turkey, in 2013. He is currently pursuing the Ph.D. degree with the CEMMETU Research Group, Middle East Technical University, Ankara. His current research interests include fast and accurate algorithms, parallel programming, broadband algorithms, integral equations, optimizations, optical metamaterials, and plasmonic materials. Karaosmanoğlu was a recipient of the 2015 IEEE AP-S Student Paper Competition Honorable Mention, the 2015 Leopold B. Felsen Award for Excellence in Electrodynamics, and the 2016 URSI-TR Best Student Paper Award.

Özgür Ergül is an Associate Professor in the Department of Electrical and Electronics Engineering at Middle East Technical University (METU), Ankara, Turkey. He is the Principal Investigator of the CEMMETU research group (http://cem.eee.metu.edu.tr). His research interests include fast and accurate algorithms for the solution of electromagnetics problems involving large and complicated structures, integral equations, iterative methods, parallel programming, and high-performance computing. He is a recipient of the 2007 IEEE Antennas and Propagation Society Graduate Fellowship, 2007 Leopold B. Felsen Award for Excellence in Electrodynamics, 2010 Serhat Ozyar Young Scientist of the Year Award, 2011 URSI Young Scientists Award, 2013 Science Academy Young Scientists Award, the first ever (2013) ACES Early Career Award, 2013 Parlar Foundation Research Incentive Award, 2014 Parlar Foundation Instructor of the Year Award, 2014 METU Young Scientist Award, 2014 TUBITAK Incentive Award, 2015 Turkish Academy (TUBA) Young Scientist Award, and 2017 IEEE Turkey Section Research Incentive Award. He is the author of the undergraduate textbooks "Guide to Programming and Algorithms Using R" (Springer) and "Introduction to Electrical Circuit Analysis (Wiley)", co-author of the graduate textbook "The Multilevel Fast Multipole Algorithm (MLFMA) for Solving Large-Scale Computational Electromagnetics Problems" (Wiley-IEEE), and coauthor of 300 journal and conference papers. He is also serving as an Associate Editor of IEEE Antennas and Propagation Magazine (Open Problems in CEM Column), a Column Editor of the URSI Bulletin (Solution Box), and an Editorial Board Member of the Scientific Reports (Nature Publishing Group). Ergül is the Chair of the IEEE AP/MTT/EMC/ED Turkey chapter and the Editor-in-Chief of Turkish Journal of Electrical Engineering and Computer Sciences (a multidisciplinary SCI-E journal).