A Spectral Integral Method for the Analysis of Nano Wires

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Abstract

This work presents a spectrally accurate method for electromagnetic scattering from objects with complex permittivity embedded in a layered medium. Two-dimensional (2D) layered medium Green's functions are computed adaptively by using Gaussian quadratures. The singular terms in the Green's functions and the non-smooth terms in their derivatives are handled appropriately to achieve exponential convergence. Numerical results, compared with the ones obtained by using other methods, demonstrate the spectral accuracy and high efficiency of the proposed method.

1 Introduction

Recently, metal and carbon nano wires (NWs) have received a serious amount of interest due to their potential in confining light transversally to sub-wavelength dimensions and yet to be used as an optical waveguide or an antenna in the visible [1]. Oulton et al. has shown that a hybrid optical waveguide, which consists of a dielectric NW separated from a metal surface by a nano scale dielectric gap, can provide extremely long propagation length (dozens of wavelengths) and strong mode confinement [2]. Experimental and theoretical results reveal a huge potential for realistic nano scale semiconductor-based plasmonics and photonics. This is why it is extremely important to develop efficient and robust algorithms for the analysis and design of such structures, especially for the ones embedded in a layered medium.

In [3], Hochman and Leviatan developed a source model technique for the analysis of NW chains. They calculated periodic Green's functions analytically as a sum of Floquet harmonics and determined the complex propagation constants of the NW chain modes directly and accurately. Their approach is mathematically correct but requires at least 10 current filaments per wavelength in order to obtain accurate results. More importantly, their approach assumes a homogeneous background, so cannot handle NWs embedded in a multilayered medium, which is a more realistic scenario. This problem can be solved more efficiently using a spectrally accurate algorithm, namely Spectral Integral Method (SIM). SIM is related to the fast method originally developed by Bojarski [4] for sound-soft circular cylinders, and extended by Hu [5] to sound-soft or sound-hard smooth cylinders. Liu et al. developed its surface integral equation solver version for homogeneous background [6] and Simsek et al. brought similar approach for multilayered background for microwave problems. The idea behind this method is the use of fast Fourier transform (FFT) algorithm and the subtraction of singularities in Green's functions to achieve a spectral accuracy in the integral. In this work, we further improve SIM to handle 2D optical scattering problems with materials and/or layers of negative permittivity. To describe the metals in the visible, Lorentz-Drude model is implemented.

2 Spectral Integration Method for Layered Media

Consider a general multilayered medium consisting of N layers separated by $N-1$ interfaces parallel to the x axis. Layer i ($i = 1, \cdots, N$) exists between $y = y_i$ and y_{i-1} ($y_0 \to -\infty$ and $y_N \to \infty$) and is characterized by relative complex permittivity $\tilde{\epsilon}_{r,i}$ and relative permeability $\mu_{r,i}$; the wavenumber inside the layer is given by $k_i = \omega\sqrt{\tilde{\epsilon}_i \mu_i}$. Assume that the scatterer is a homogeneous object residing in several layers of

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the background. The boundary of the scatterer is described as $r = r(\theta)$, or equivalently $[x = x(\theta), y = y(\theta)]$ in terms of a parameter θ (in this case the azimuthal angle $\theta \in [0, 2\pi]$). An incident TM_z wave is assumed and the time dependence of $e^{j\omega t}$ is implied.

For the TM_z case, the 2D Helmholtz equation for the scalar field E_z is

$$\nabla \cdot \mu_{r,\gamma}^{-1} \nabla E_z + k_0^2 \tilde{\epsilon}_{r,\gamma} E_z = -f_\gamma \tag{1}$$

where subscript γ indicates the region outside ($\gamma = l$) or inside ($\gamma = d$) the object, f_γ is the source excitation, $k_\gamma = \omega\sqrt{\mu_\gamma \tilde{\epsilon}_\gamma}$, and $k_0 = \omega\sqrt{\mu_0 \epsilon_0}$. For a smooth dielectric object embedded in a layered medium, one boundary integral equation on the outside of surface of the scatterer D can be obtained as

$$E_z^{inc}(\mathbf{r}) + \oint_D \left[\frac{\partial E_z(\mathbf{r}')}{\partial n'} G_l(\mathbf{r}, \mathbf{r}') - E_z(\mathbf{r}') \frac{\partial G_l(\mathbf{r}, \mathbf{r}')}{\partial n'} \right] ds' = \frac{E_z(\mathbf{r})}{2} \tag{2}$$

for $\mathbf{r} \in D$, where f_d is assumed zero, E_z^{inc} is the incident wave from outside the object (i.e., $f_l \neq 0$, $f_d = 0$), $\hat{\mathbf{n}}$ is the outward unit normal, and $G_l(\mathbf{r}, \mathbf{r}')$ is the layered-medium Green's function given by

$$G_l(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi} \int_0^\infty \tilde{G}(k_x, y|y') \cos k_x(x - x') dk_x, \tag{3}$$

where $\tilde{G}$ is the spectral domain counterpart. $G_l(\mathbf{r}, \mathbf{r}')$ can be written as

$$G_l(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi} \int_0^\infty \left[\tilde{G}(k_x, y|y') - \tilde{G}_{sub}(k_x, y|y') + \tilde{G}_{sub}(k_x, y|y') \right] \cos k_x(x - x') dk_x, \tag{4}$$

where

$$\tilde{G}_{sub}(k_x, y|y') = \frac{\mu_{r,m}}{2jk_{x,m}} e^{-jk_{x,m}|y - y'|}, \tag{5}$$

and $\mu_{r,m}$ is the m^{th} layer's relative permeability where the field point is, and $k_{x,m}^2 = k_m^2 - k_x^2$. Finally, (3) can be written as

$$G_l(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi} \int_0^\infty \left[\tilde{G}(k_x, y|y') - \tilde{G}_{sub}(k_x, y|y') \right] \cos k_x(x - x') dk_x + \frac{\mu_{r,m}}{4j} H_0^{(2)}(k\rho), \tag{6}$$

where $\rho = \sqrt{(x - x'^2) + (y - y')^2}$, and $H_0^{(2)}$ is the zeroth order Hankel function of the second kind. This formulation is the same as the primary field term subtraction when source and field points are in the same layer [9],[10]-[8]. The important caution is that this subtraction procedure is used even if the source and field points are in different layers. Hence, we can seperate the layered media Green's function into two parts: singular and nonsingular. As described in [5], we can define an infinitely smooth function to handle the singular behavior in terms of θ as follows

$$\hat{G}_l(\theta, \theta') \equiv G_l(\theta, \theta') + \frac{1}{2\pi} \ln \left| 2 \sin\left(\frac{\theta - \theta'}{2}\right) \right| J_0(k_{l,m} R). \tag{7}$$

Similar procedure follows for the derivative of the Green's function, $\partial G_l(\mathbf{r}, \mathbf{r}')/\partial n'$, as described in [9] not only for the primary field term but also for reflection terms.

The unknown field and its derivative can be approximated by truncated Fourier series in terms of θ along the boundary of the scatterer. Then the two integrations in Eq. (2) can be calculated using FFT with high accuracy. After collocation at $\{\theta_m\}$ points, Eq. (2) can be written in a compact form as follows

$$L\tilde{\mathbf{e}}_z^b + M\tilde{\mathbf{h}}_t^b = \mathbf{E}_z^{inc} \tag{8}$$

where $\tilde{e}_{zn}^b$ and $\tilde{h}_{tn}^b$ are the Fourier's coefficients of $E_z(\theta')$ and $\frac{\partial E_z(\theta')}{\partial n'}$, respectively, N_s is the number of discretized Fourier transform points; $L_{mn} = e^{jn\theta_m}/2 + 2\pi h_{mn} + k_b v_{mn}$ and $M_{mn} = -2\pi g_{mn} + u_{mn}$ in which $m, n = 1, 2, \cdots, N_s$, are the indices of basis and testing points on the discrete boundary; g_{mn} and h_{mn} are

Fourier transforms of the smooth parts, and u_{mn} and v_{mn} are Fourier transforms of the two non-smooth terms of the Green's function and its normal derivative (see [9] for the expressions). Because of the use of singularity subtraction and FFT, the calculations of these terms are convergent, fast, and have high accuracy. The second boundary integral equation for the interior problem can be discretized in the same way. The final form of the equations can be solved for the scalar field (E_z) and its normal derivative ($\partial E_z/\partial n'$) on the boundary of the scatter. From the solution of these field variables on the boundary, the fields everywhere can be obtained by the Green's theorem.

3 Lorentz-Drude Model

In order to define metals in visible, Lorentz-Drude model is implemented. For gold, ϵ_∞ is assumed to be 1 and plasmon frequency, ω_p, is taken as 9.03ζ, where $\zeta = e/\hbar = 1.51925 \times 10^{15}$ Hz. Then, frequency dependent complex permittivity of gold is calculated using

$$\epsilon(\omega) = \epsilon_\infty + \sum_{k=1}^{k=6} \frac{a_k \omega_p^2}{\omega_k^2 - \omega^2 - i b_k \omega} \tag{9}$$

where

k	1	2	3	4	5	6
a_k	0.760	0.024	0.010	0.071	0.601	4.384
b_k/ζ	0.053	0.241	0.345	0.870	2.494	2.214
ω_k/ζ	0.000	0.415	0.830	2.969	4.304	13.32

4 Numerical Results

To show the accuracy and efficiency of the method, a circular gold object in free space is chosen as the first example as it has an analytical solution. An infinite gold circular cylinder with radius $r = 300$ nm is excited with a TM$_z$ plane wave at $\lambda = 600$ nm impinging at an angle $\theta^{inc} = 0°$ along the x-direction. According to Eqn. (9), complex relative permittivity of gold at given wavelength is equal to -7.9877 +i2.0623. The receiver points are chosen along the $-\lambda < x, y < \lambda$. Figure 1 shows the comparison between the SIM result and analytical solution for the scattered field. For this example, 64 points along the boundary of the object are used, and excellent agreement has been observed. In the next step, we change the number of samples

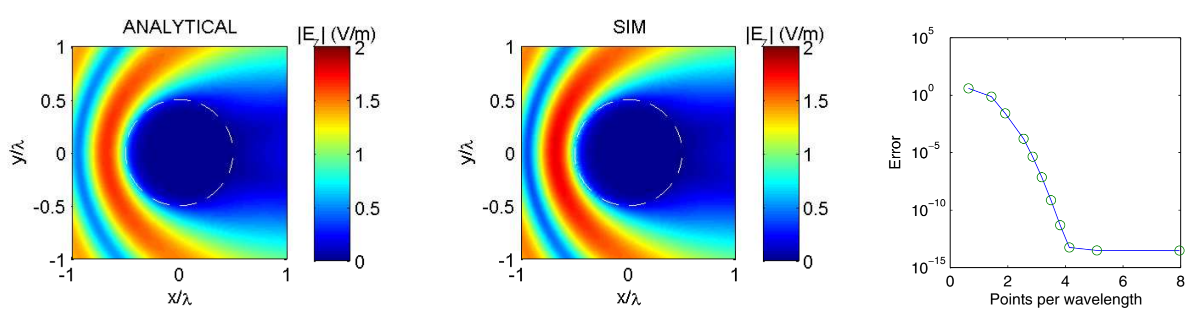

Figure 1: Comparison of the analytical (left) and SIM (middle) results for a gold cylinder situated in vacuum. Diameter of the cylinder is $R = \lambda = 600$ nm. $\epsilon_{gold} = -7.9877 + i2.0623$ for the given wavelegnth. White dashed line depict the location of the gold cylinder. (Right) Error versus the number of discretization points per wavelength.

taken on the boundary in order to observe the proposed method's overall accuracy. On the right of Figure

1, we plot the error convergence curve versus the number of discretization points per wavelength (PPW) on the object. The error decreases exponentially with the number of discretization points, confirming that the SIM has a spectral accuracy. The result shows that even with a small discretization number (such as 3 PPW) on the boundary of the cylinder, the relative error is smaller than 1 %.

At the conference, we will also provide examples where the infinite cylinder embedded in a multilayered medium, which are not provided here for the sake of brevity.

5 Conclusion

We further improved the spectral integral method for homogeneous objects with complex permittivity and closed smooth boundary. The high accuracy and the efficiency of the method has been demonstrated. 1% accuracy can be obtained with about three points per wavelength sampling. Numerical results also confirm that the SIM is applicable to concave objects. The method can be further extended to periodic structures and to three dimensions, as well as to objects traversing layer interfaces.

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