Analysis of photonic structures in layered geometries by MMP

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Summary. In this work, a numerical analysis method is introduced by combining the Multiple Multipole Program (MMP) and layered geometry Green's functions. By the method, several difficulties in the analysis of photonic structures in layered geometries are eliminated and an efficient simulation tool is obtained that can analyze both $2D$ and $3D$ geometries.

1 Introduction

The advancements in the fabrication process of photonic structures, made various nano devices quite popular, including photonic crystals, chemical and bio sensors, optical antennas and waveguides [1]. Mostly, these photonic devices are fabricated in a multilayered structure. In the numerical analysis of such structures, the layers are often ignored for the sake of simplicity of simulations, which can cause substantial inaccuracies in the results. Especially for structures that support Surface Plasmon Polariton (SPP) or guided wave modes, the errors become so high that the computations become useless. In order to understand the physical phenomena related to layered geometries and to improve the efficiency of the devices, a numerical analysis tool that takes the layered geometries into account efficiently is needed. In this paper, a candidate for such a numerical tool is introduced by combining MMP and layered media Green's functions.

2 The Method

Since the main idea of the method introduced, is to combine MMP and layered media Green's functions, both of them will be discussed briefly below.

2.1 MMP

MMP is one of the most reliable and efficient computational tools for the analysis of plasmonic structures in frequency domain [2]. It is a semi-analytical, boundary discretization method that uses various analytic solutions of the Maxwell equations or so called expansions (e.g. plane waves, cylindrical waves, spherical waves, etc.) in order to approximate the fields scattered by the objects. In the MMP analysis, the electromagnetic field in domain i (F^i) can be written as a superposition of the fields generated by the expansions as:

$$F^i = \sum_{n=1}^{N_i} A_n^i E_n^i + \mathbf{error} \tag{1}$$

where E_n^i is the field generated by expansion n and A_n^i is the corresponding complex amplitude. The amplitudes are computed in such a way that the weighted residuals are minimized on the interfaces between different domains.

2.2 Layered media Green's functions

The Green's function describes the field generated by an infinitesimal source at a ceratin location. In free space, the Green's function can be represented by closed form formulations (1D (an infinitely large plane is the source): plane wave, 2D (an infinitely long line is the source): cylindrical monopole waves, 3D (a point is the source): spherical dipole waves), which makes it easy and fast to use them as expansions in methods such as MMP or Method of Moments (MoM). In the case of a layered geometry, the Green's functions can only be obtained by summing up all the plane waves that are generated at the location of the point source, for which the continuity conditions between different layers are fulfilled analytically. Since the spectrum of a point source is continuous (i.e. all the propagating and evanescent plane waves should be taken into account), the summation leads to an integral (Sommerfeld integral) with infinite bounds as follows (when the layers are stacked in y-direction and $e^{-i\omega t}$ is used):

$$G(x,y,z) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dk_z dk_x e^{ik_z z} e^{ik_x x} \tilde{G}(k_x,k_z) \tag{2}$$

where $G(x,y,z)$ and $\tilde{G}(k_x,k_z)$ are the spatial and spectral domain Green's functions for the given field component, respectively. In this calculation, the reflection and the transmission relations for the given plane wave is contained in the spectral domain Green's function [3]. In general, the integrands of (2) are oscillatory and slowly decaying which makes the integration numerically expensive. This burden can be handled by using series acceleration techniques. In this work, the Aitken series and weighted averages methods are used in order to decrease the time needed for the integrations [4].

Equation (2) is the most general form of the Sommerfeld integral, which provides the Green's function in 3D. One can obtain the Green's function in 2D by (2), e.g., by taking the k_z value as a constant for a line source in z-direction. It is also possible to obtain the Green's function of a complex origin source which generates beams by changing the integration paths, so that the integrands stay stable. This kind of expansions can be used to decrease the total number of expansions, especially for long structures compared to the wavelength.

By using layered media Green's functions as an expansion set in MMP, one can decrease the complexity of the problems, since the continuity conditions on the layered geometry is fulfilled analytically [5]. In the next section, numerical examples will follow, demonstrating the efficiency of the method.

3 Numerical Examples

As the first example, a $2D$ triangle scatterer is placed in a four layered geometry. The result of the simulation, and the problem specifications are given in Fig. 1. For this simulation, a total of 76 expansions (38 for the field inside the scatterer (free space monopoles) and 38 for the field outside the scatterer (layered expansions)) are used, which makes the maximum relative error on the interface of the scatterer $\sim 0.1\%$. For this problem, since the incident field does not propagate in z-direction ($k_{z,inc} = 0$), the layered expansions are obtained by (2) with $k_z = 0$.

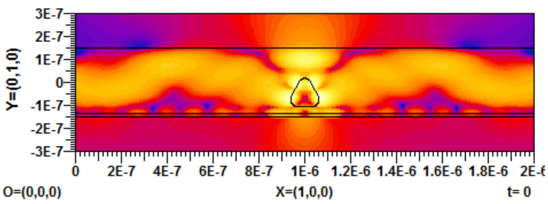

Fig. 1. Scattered field, magnitude of H_z component in logarithmic scale. Incident field: H_z polarized plane wave impinging normally on top of the structure with $\lambda_0 = 600nm$. Layer-1(lowermost layer) and Layer-4(uppermost layer) are free-space, Layer-2: Ag ($\varepsilon_{r2} = -15.91 + i0.43$) $d_2 = 15nm$, Layer-3: dielectric material ($\varepsilon_{r3} = 9.0$) $d_3 = 285nm$. The scatterer is Ag elevated $50nm$ from the boundary between layers 2 and 3. The side lengths of the scatterer are 160, $160\sqrt{5}$ and $160\sqrt{5}nm$ with the rounding radius of $30nm$.

For the second example, an Ag sphere in a dielectric slab sitting above an Ag substrate is analyzed. For this simulation, 73 expansions (1 for the field inside the sphere (free-space multipole with max. order and degree of 5) and 72 for the field outside the sphere (layered expansions)) are used resulting in a maximum relative error of $\sim 0.1\%$. The result and the problem specifications are given in Fig. 2.

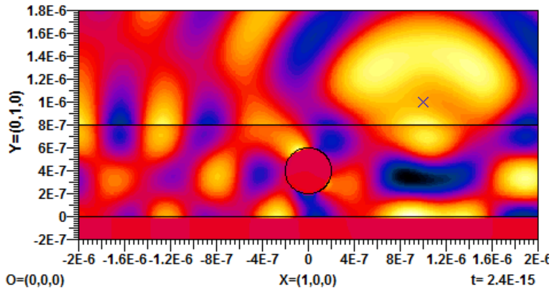

Fig. 2. Total field, E_y component at an instance of time on XY-plane ($z = 0$). Incident field: Vertical electrical dipole at $(1,1,1)\mu m$ $\lambda_0 = 750nm$. Layer-1(lowermost layer): Ag ($\varepsilon_{Ag} = -26.73 + i0.33$), Layer-2: dielectric material ($\varepsilon_{r2} = 9.0$) $d_2 = 800nm$ and Layer-3(uppermost layer) is free-space. The scatterer is an Ag sphere with $r = 200nm$ located at the center of Layer-2.

4 Conclusion

In this paper a numerical tool is introduced by combining layered media Green's functions and MMP. As a result, an efficient tool is obtained that can solve the scattering problems in 2D and 3D geometries.

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