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Modelling of a single object embedded in a layered medium

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We present a numerical method based on the method of the fictitious sources to model one or several inclusions of arbitrary shape in stratified media. Our aim is to propose an efficient numerical method for the modelling of plasmonic devices. Indeed, metals impose rapid decays of the electromagnetic fields that are often a problem for methods based on a volume meshing. We give the theoretical basis of the method and also some practical details of its implementation in order to obtain an efficient numerical code. The efficiency of the numerical code is illustrated by modelling a spherical open cavity in a metal layer and a hole in a dielectric layer.

1. Introduction

The research field that is known as plasmonics is nowadays highly topical [1, 2]. This field can be defined as being based on the use of surface and particle plasmon resonances of noble metal in optics. Metals have long been considered as materials that suffer from important losses and thus, whose range of application in optics is limited. However, researchers have realized that one key issue in the domain of nanophotonics would be the ability to control light at scales considerably smaller than the wavelength. One of the major issues would be to tailor molecule emission [3]. With respect to this aim the localized plasmons of particles have attractive characteristics. Even waveguides would be of interest if one wants to integrate optical circuits with a higher density than with dielectrics [4]: the short propagation distance would compensate the propagation losses.

Modelling with metals in optics has always been confronted with the difficulty that the fields experience a rapid spatial exponential decay. Thus any numerical method based on a regular mesh of space would face the dilemma that the mesh should be fine enough to sample exponential decay but the number of unknowns cannot be indefinitely increased due to computational time and available memory on computers. Methods such as finite time domain differences, differential method of

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the grating theory, coupled dipole method and numerous others are all plagued by this problem.

Another class of method is based on the assumption that the permittivity and permeability of the objects are piecewise constant; i.e. the object is made of homogeneous materials. It is well known that under this assumption it is possible to transform the original volume problem into a surface problem [5]. One example of this type of method is the surface integral method widely used for the modelling of gratings [6], rough surfaces [7], etc.

In this paper we will consider another approach that was developed in the late 1980s by several groups and known as the multiple multipole method [8], method of fictitious sources (MFS) [9] or method of auxiliary sources [10]. Historically the first attempts to use this method in electromagnetism are due to Kupradze [11]. The method has been applied to several problems, including grating modelling [9], photonic crystals design [12], etc. The interested reader can find in a recent review article many developments of the methods that have been proposed since the original pioneering work [13].

Our aim is to apply the method to the problem of a single inclusion of arbitrary shape embedded in a stratified media. One of the main applications envisaged is the modelling of a single hole in a metallic film that has been a subject of interest in the last few years [14, 15] and whose modelling still deserves some additional work. For example, the shape of the cross-section of a single hole, the local density of states or the emission of an atom located in the hole are still to be theoretically investigated.

2. The method of fictitious sources: from a volume problem to a surface one

The basic idea of the method is that the field in a given medium (homogeneous or stratified) can be represented by a sum of fields radiated by appropriate fictitious sources located outside the considered medium. The exact location and the nature of these sources can be chosen almost freely. It gives to the method an important flexibility, but the numerical efficiency is dependent on the choices. The fictitious sources have no physical meaning and can be seen as a natural extension of the secondary sources introduced by Huygens and taken up later by Fresnel [16].

Our approach relies on unquestionable theorems of functional analysis. For conciseness, this aspect is not developed here, but the interested reader can refer to [17].

Let us consider a diffraction problem by a 3D bounded homogeneous object whose boundary is a closed surface $\mathcal{C}$ (figure 1) embedded in a stratified media. We assume that $\mathcal{C}$ is of class C^2, and we denote by $\hat{\mathbf{n}}$ the unit vector of the outward normal. We call Ω_1 and Ω_2 the exterior and interior domains of $\mathcal{C}$. The domain Ω_2 is filled with a material of permittivity ε_2 which is complex with a positive imaginary part, while the domain Ω_1 is filled with a stratified medium, i.e. a medium made of a finite number of homogeneous layers. The interfaces of the layers are assumed to be perfectly plane and parallel to the xOy plane. In the sequel, F and F^{inc} will be used as short notations for the components of both electric and magnetic fields. A known

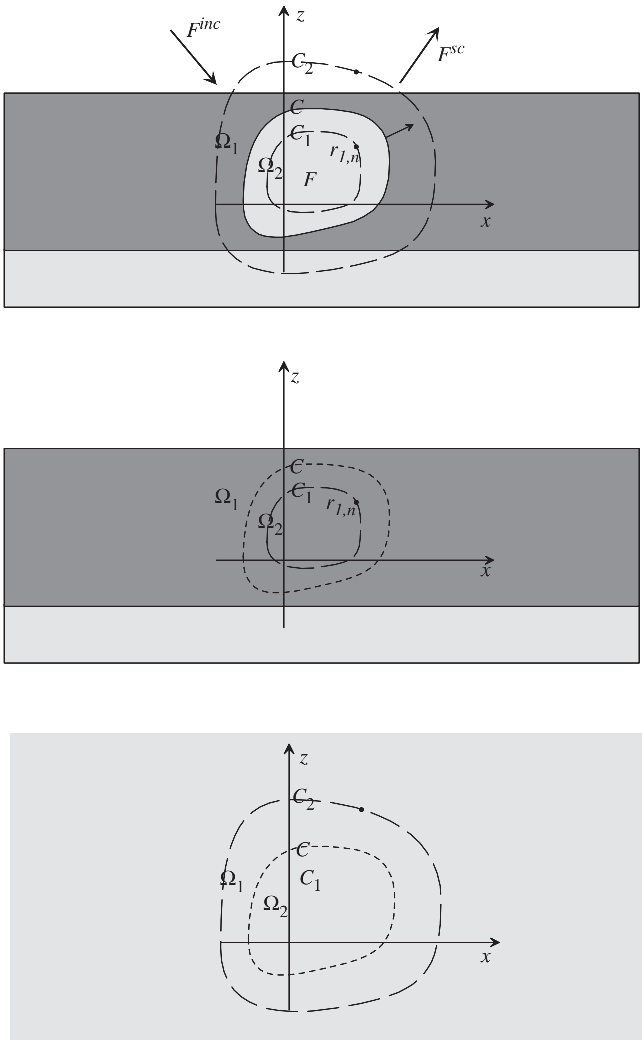

Figure 1. Top: schematic representation of the problem. The light grey object is lying in a stratified medium made of two layers that are assumed to be infinite along the x axis and the y axis. Middle: the fictitious sources inside the object are located on $\mathcal{C}_1$ and radiate in the stratified medium surrounding the object. Bottom: the fictitious sources outside the object are located on $\mathcal{C}_2$ and radiate inside the homogeneous medium filling the object.

incident field $F^{\text{inc}} = (\mathbf{E}^{\text{inc}}, \mathbf{H}^{\text{inc}})$ illuminates the object, and we look for the total field $F = (\mathbf{E}, \mathbf{H})$. From the Stratton–Chu formulae [5], it turns out that the electromagnetic field at any point can be deduced from the values of $\hat{\mathbf{n}} \times \mathbf{E}$ and $\hat{\mathbf{n}} \times \mathbf{H}$ on $\mathcal{C}$. Thus we will represent the field by the couple Φ of vector functions defined on $\mathcal{C}$, which is the unknown of the problem (η_0 is the vacuum impedance):

$$\Phi = (\hat{\mathbf{n}} \times \mathbf{E}, \hat{\mathbf{n}} \times \eta_0 \mathbf{H}). \tag{1}$$

In the same way, the incident field can be represented by the couple of functions Φ^{inc} defined on $\mathcal{C}$:

$$\Phi^{\text{inc}} = (\hat{\mathbf{n}} \times \mathbf{E}^{\text{inc}}, \hat{\mathbf{n}} \times \eta_0 \mathbf{H}^{\text{inc}}). \tag{2}$$

Let us define the scattered field F^{sc} as the difference between the actual total field and the incident field:

$$F^{\text{sc}} = F - F^{\text{inc}}. \tag{3}$$

A simple way to understand the method is to keep in mind that the problem is to find the total field F such that:

(a) the scattered field F^{sc} satisfies Maxwell's equations in Ω_1 and a radiation condition at infinity,
(b) the total field F satisfies Maxwell's equations in Ω_2,
(c) the boundary conditions on the surface $\mathcal{C}$ of the scatterer are fulfilled.

Let us consider sources $S_{1,n}$ ($n = 1, 2, \ldots, N$) placed in Ω_2 and which radiate fields $F_{1,n} = (\mathbf{E}_{1,n}, \mathbf{H}_{1,n})$ in the whole space supposed to be filled with the stratified media (see figure 1). Since the sources are placed in Ω_2, $F_{1,n}$ has no singularity in Ω_1 and $F_{1,n}$ verifies condition (a) above. Any linear combination $\sum_n c_{1,n} F_{1,n}$ will also fulfil condition (a) and, for well chosen $c_{1,n}$, this series can be regarded as an approximation for F^{sc} in Ω_1. In the same way, we consider sources $S_{2,n}$ placed in Ω_1 and radiating fields $F_{2,n}$ in the whole space supposed to be filled with the material of permittivity ε_2. A linear combination $\sum_n c_{2,n} F_{2,n}$ of such fields fulfils condition (b) and, if the $c_{2,n}$ are well chosen, can be regarded as an approximation for F in Ω_2. Denoting by $\Phi_{1,n}$ and $\Phi_{2,n}$ the boundary values of the fields $F_{1,n}$ and $F_{2,n}$ on $\mathcal{C}$, the continuity of the tangential components of the total field on $\mathcal{C}$ (condition (c)) reduces to

$$\Phi^{\text{inc}} + \sum_n c_{1,n} \Phi_{1,n} - \sum_n c_{2,n} \Phi_{2,n} = 0. \tag{4}$$

From a theoretical point of view, one can define vector spaces for ϕ, Φ^{inc}, $\Phi_{1,n}$ and $\Phi_{2,n}$.

Thus, equation (4) is noting the decomposition of ϕ on two bases $\Phi_{1,n}$ and $\Phi_{2,n}$ according to

$$\Phi = \Phi^{\text{inc}} + \lim_{N\to\infty} \sum_{n=1}^{N} c_{1,n}(N) \Phi_{1,n} = \lim_{N\to\infty} \sum_{n=1}^{N} c_{2,n}(N) \Phi_{2,n}. \tag{5}$$

Note that the norm defined in this vector space involves surface integrals on $\mathcal{C}$ of the tangential components of the fields F^{inc}, $F_{1,n}$, $F_{2,n}$ (the definition of the norm being necessary to define the convergence in equation (5)).

Obviously numerical computations will necessarily involve a finite set of sources and thus an incomplete base. Thus, for a number N of sources, the aim is to get the coefficients $c_{1,n}$ and $c_{2,n}$ (depending on N) which give the following norm its minimum value Δ_N:

$$\Delta_N = \min \left\| \Phi^{\text{inc}} + \sum_{n=1,N} c_{1,n}(N) \Phi_{1,n} - \sum_{n=1,N} c_{2,n}(N) \Phi_{2,n} \right\|. \tag{6}$$

Once the coefficients $c_{1,n}$ and $c_{2,n}$ are known, the field in each region is given by

$$F^{sc} \approx \sum_{n=1,N} c_{1,n} F_{1,n} \quad \text{in } \Omega_1 \tag{7}$$

and

$$F \approx \sum_{n=1,N} c_{2,n} F_{2,n} \quad \text{in } \Omega_2. \tag{8}$$

Note that a problem involving several inclusions can be modelled by adding a set of sources for each and fulfilling the boundary conditions on each.

In the numerical implementation we use a least-squares algorithm in order to minimize the norm (6) that has two interesting features. First, it allows us to use non-square systems and to obtain a better accuracy for an identical computational burden. Second the normalized error $\tilde{\Delta}_N = \Delta_N / \|\Phi^{inc}\|$ provides a good criterion on the precision of the solution.

3. Examples

To illustrate the method we will consider two different structures.

The first example consists of a spherical open cavity in a metallic layer. Similar cavities have been realized and characterized recently [18, 19]. Here we will consider a single cavity, while in the experiments the cavities were arranged in arrays but could be considered as isolated cavities. From the modelling point of view it could be seen as a spherical inclusion (made of vacuum) in a stratified medium. Here we have considered a sphere of radius 350 nm whose centre is at $x = y = z = 0$ and the stratified medium is made of a single metal layer whose permittivity is $-9.89 + 1.05i$ and its interfaces are parallel to the x–y plane and located at $z = -400$ nm and $z = +200$ nm. Both substrate and superstrate are assumed to be in vacuum. Note that given the radius of the sphere, it overlaps with the metal layer and the superstrate, thus the cavity is open on its upper side.

The fictitious sources used to solve this problem are of two different natures. The fictitious sources located outside the spherical inclusion are assumed to radiate in the homogenous medium filling the inclusion (i.e. vacuum). In our case we have chosen to make use of dipoles. On the other hand, the sources located inside the inclusion are assumed to radiate in the stratified medium (but without the inclusion). Here again we considered dipoles but as the environment is no longer homogenous the radiated field is no longer given in a closed form. We used the method proposed by Martin and co-workers [20] and extended it to the computation of the magnetic field (as the tangential components of the magnetic field on the inclusion are also required). A repartition of sources on spheres of radius 245 and 455 nm (resp. for the internal and external sources) has been found to give accurate results for reasonable computational burden. We used 640 fictitious sources on each sphere (two crossed dipoles on each of the 320 points on the spheres) and the boundary conditions are computed on 500 points on the spherical inclusion. With this configuration we have about one point for each $(\lambda/15)^2$ area on the spherical inclusion. Thus, the

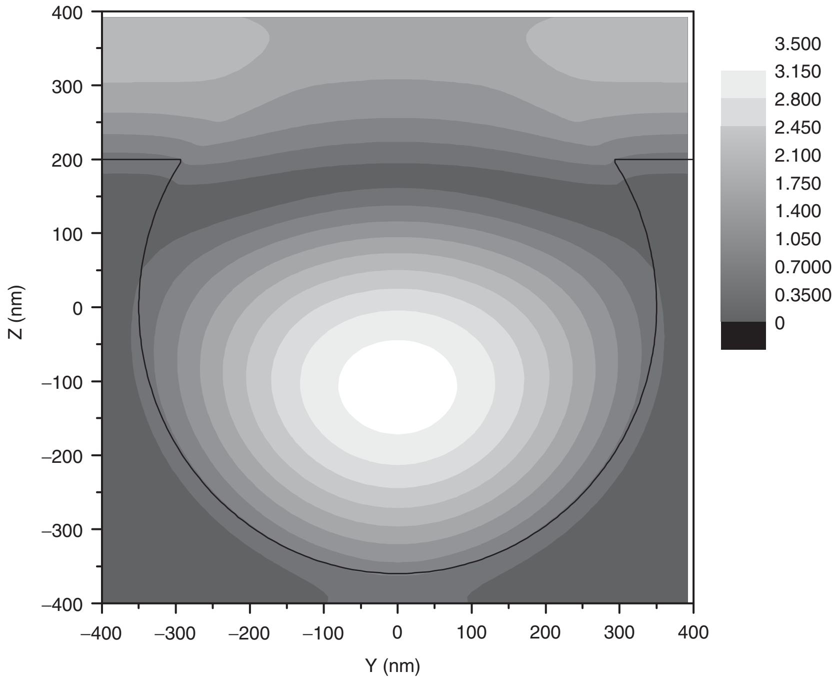

Figure 2. Modulus of the electric field in a nanocavity made of a spherical void inclusion in a metallic (gold) layer. The structure is assumed to be illuminated by a plane wave propagating in the $-z$ direction, polarized along the x axis and with a wavelength equal to 800 nm.

least-squares problem consists in minimizing the error on the continuity of the two tangential components of the electric and magnetic fields on 500 points (i.e. 2000 equations) by choosing 1280 amplitudes of the fictitious sources.

From a practical point of view the objects (inclusion and fictitious surfaces) are meshed using conventional free or commercial software. Indeed the only requirement is to have regularly spaced points and the normal to the surface at these points. The use of standard software allows us to model a particle of any shape.

Figure 2 shows a map of the modulus of the electric field when the structure is illuminated by a plane wave coming from the top of the figure, with a normal incidence (with respect to the stratified media), linearly polarized along the x axis and a wavelength equal to 800 nm. The enhancement of field inside the cavity shows that a resonance of the cavity has been excited, but note that the parameters have not been optimized with this aim.

In order to illustrate that point we have plotted on figure 3 the residual error on each point of the embedded object. Note that the error is always less than 9×10^{-2}.

The second example is a single hole in a dielectric layer surrounded by air. The hole is assumed to be invariant along z and has a circular cross-section with radius 50 nm. As the structures we have in mind to model are nano-holes or nano-objects for optical applications this is not really a limitation and is realistic for actual devices. The thickness of the layer is 160 nm and the permittivity is 2.25.

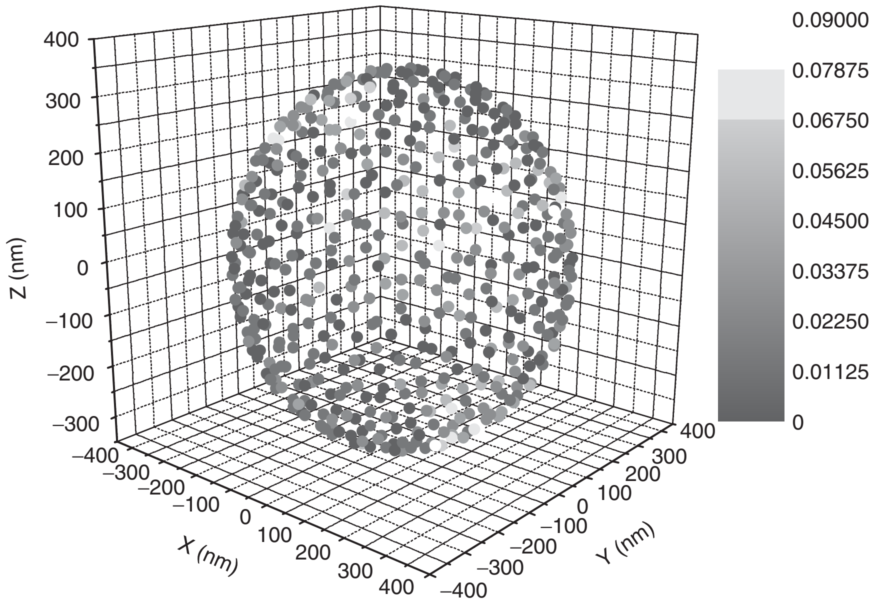

Figure 3. Normalized residual error on the boundary conditions. Each point on the sphere inclusion has a greyish tinge given by the normalized error on the point.

The considered wavelength is 400 nm. Note that the embedded object is a cylinder whose edges have been rounded with a radius of 20 nm (the total height of the rounded cylinder is 200 nm, see white dashed line in figure 4). The exact location and shape of the upper and lower faces of the cylinder does not change the results as the hole is assumed to be filled by air as are the substrate and superstrate, but it allows us to avoid sharp edges that may cause numerical instabilities. We have checked that 1632 sources and 800 points on the object give satisfactory results. Figure 4 shows the map of the modulus of the electric field when the structure is illuminated by a plane wave incident from the top with normal incidence and linearly polarized along the x axis.

4. Conclusion

We have presented an extension of the method of the fictitious sources to one or several inclusions of arbitrary shape in stratified media.

We have sketched the theoretical basis of the method and given some practical details of its implementation in order to obtain an efficient numerical code. The method has been illustrated by modelling a metallic nanocavity made of a spherical void inclusion in a metallic film and a circular hole in a dielectric layer.

Our aim in developing this method was to provide an efficient numerical tool for modelling in the domain of plasmonics. Indeed, one of the main advantages of the method is that the problem amounts to seeking the tangential components of the

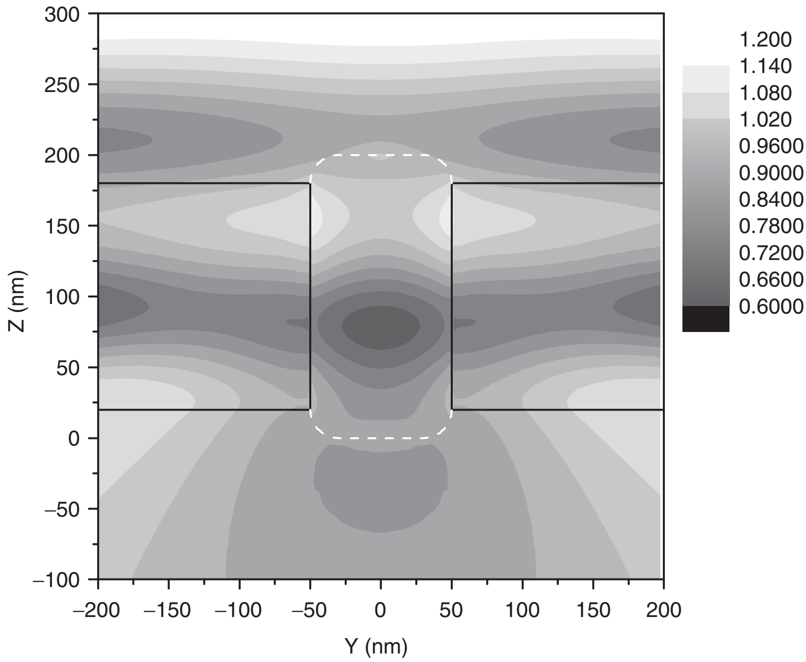

Figure 4. Modulus of the electric field in a hole in a dielectric layer. The structure is assumed to be illuminated by a plane wave propagating in the – direction, polarized along the x axis and with a wavelength equal to 400 nm.

fields on the boundaries of the inclusion. Thus, contrarily to the methods using a volume mesh we will not face very fine meshing due to the exponential decay of the fields in the metals. Among the phenomena we envisage to model, extraordinary transmission through subwavelength single holes comes first. The method would also be of interest in a variety of topical problems in optics such as laser damage due to local defects in thin film optical components, sensors based on particle plasmon resonances or the role of the shape of particles in giant Raman scattering.

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