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A New Guideline for the Allocation of Multipoles in the Multiple Multipole Method for Two Dimensional Scattering from Dielectrics

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ABSTRACT

A new guideline for proper allocation of multipoles in the multiple multipole method (MMP) is proposed. In an 'a posteriori' approach, subspace fitting (SSF) is used to find the best location of multipole expansions for the two dimensional dielectric scattering problem. It is shown that the best location of multipole expansions (regarding their global approximating power) coincides with the medial axis of the object. The subspace analysis is performed for various scenarios including objects with different shapes and sizes relative to the wavelength, different permittivities and both TE_z and TM_z polarizations. Numerical examples for both TE_z and TM_z cases are also presented. The results are in a very good agreement with the finite element method (FEM) results. Two challenging test cases are presented. First, a large object compared to the wavelength and second, a small object with field singularities close to the boundary. Accuracy of the final MMP results shows the effectiveness of the new allocation rule.

KEYWORDS

Multiple Multipole Method, Subspace Analysis, Electromagnetic Scattering.

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1- INTRODUCTION

Computational electromagnetics has played a key role in the development of emerging technologies in the past three decades [1]. One important area of research for these developments is the analysis of scattering of electromagnetic waves from dielectric objects. The application areas vary greatly and include the remote sensing of buried objects [2], the microwave imaging of biological tissues [3], and the design and analysis of optical and photonic devices [1, 4].

The generalized multipole technique (GMT) is a powerful and accurate mesh-free method for solving time-harmonic electromagnetic field problems, especially for the analysis of scattering from objects with smooth boundaries [1, 4, 5, 6, 7, 8, 9]. The essence of the GMT is to approximate the solution by a finite linear combination of fields of multipole sources [10]. Additionally, due to the use of the generalized point matching [11], the GMT solutions do not involve any integration [12, 13]. One of the most popular variants of the GMT is the multiple multipole method (MMP) which is introduced by Hafner in 1980 as a generalization of the Mie theory [14]. In this method, the fields are approximated by multipole expansions about different origins [10].

A crucial step in the GMT is the allocation of approximating sources [15], which has a significant effect on the convergence and accuracy of solutions [11, 16, 17]. For the MMP, the problem of multipole placement has been addressed in several publications [7, 11, 18, 19]. Generally, the problem could be handled by either a priori or a posteriori approach. In the former approach one tries to allocate the expansions based on physical and geometrical specifications of the problem while the latter approach involves analysis of fields from previously solved problems. As an example, an optimization algorithm were proposed by Leuchtmann for the electrostatic case where multipoles were added one by one and selected iteratively by minimizing the residual error along the boundary [20]. The algorithm gives monotonically convergent results. Yet it was abandoned since its computational burden was significantly high [21]. Indeed, the optimum location depends on detailed specifications of the scattering problem such as the incident field, the object's geometry, and electromagnetic properties of the corresponding domains [7, 17, 21, 22]. Hence, determination of the best position for multipoles' origins is not trivial.

A review of previously developed allocation algorithms shows that the most effective algorithms are based on a priori approaches [7, 11, 19, 21, 18]. A good example is the geometric rules provided by Hafner [11], implemented in allocation algorithms by Regli [19], and refined for special cases by Moreno [7].

The Hafner's geometric rules of thumb rely on the so called domain of greatest influence of a multipole [11]. This domain is defined as a disk centered at the multipole's origin with its radius equal to a constant factor times the distance between the multipole's origin and the objects boundary [11]. The underlying assumption is that the behavior of multipole fields along the boundary is local, that is the amplitude of a multipole's field is negligible outside a neighborhood of origin of the multipole [23, 24]. This requires the distance between origins of multipoles and the object's boundary to be at most about one wavelength [7]. It is clear that the amplitude of multipole fields along the boundary depends on their orders too. Therefore, defining the same influence domain for multipoles with different orders reduces the robustness and reliability of the final algorithms.

Using optimization approaches it could be shown that the best location for placing a multipole inside a circular domain is at the center of the circle [21]. The solution is then identical to the Mie solution for circular cylindrical objects. However, when it comes to the scattering from non-circular boundaries, the allocation rules seem to be too heuristic without proper justification.

In this paper, by using an a posteriori approach for dealing with the allocation problem in the MMP, we introduce a simple and justified rule. The proposed guideline then could be used as a basis for algorithms in an a priori approach. Here, the expansion allocation problem is investigated in the framework of a parameter estimation method. The novel application of the subspace-fitting method to this problem reveals where the multipole subspace is best fitted to the signal space of the scattered field. The results show that for different dielectric objects a common geometric entity that coincides with the medial axis of the objects could be regarded as the desired location of multipole's origin.

The paper is outlined as follows. Section 2 includes a brief introduction of the MMP method. The subspace analysis is presented in Section 3. Different scattering problems are then solved by exploiting the proposed idea in Section 4 followed by the paper's conclusions in Section 5.

2- MULTIPLE MULTIPOLE METHOD

The general geometry of the problem for the two dimensional scattering form a single dielectric object is shown in Fig. 1. The scatterer is assumed to be linear, homogeneous and non-magnetic. Here, an object with the relative permittivity of ε_{r} is illuminated by the incident field f^{inc} in the surrounding free-space. Based on the polarization of the incident field, f^{inc} could represent either the electric field (TM_z), or the magnetic field (TE_z). Recalling that the scattered field is defined as the difference between the total field in the presence and the absence of the object, the scattering problem is to find the scattered field f^{sct} given the incident field f^{inc}.

In the MMP framework, the scattering problem is solved by approximating the scattered field exterior and the total field interior to the object by a linear combination of truncated multipole expansions [11]. Accordingly, assuming the time dependence of $\exp(j\omega t)$, the scattered field is approximated by L expansions as

$$f^{sct}(\mathbf{r}) \approx \sum_{l=1}^{L} \sum_{n=-N_l}^{N_l} a_{ln} H_n^{(2)}(k_1|\mathbf{r} - \mathbf{r}'_l|) \exp\big(jn\angle(\mathbf{r} - \mathbf{r}'_l)\big), \quad (1)$$

where $\mathbf{r}$ and $\mathbf{r}'_l$ are the position vectors of the observation point and the expansion centers, respectively; $H_n^{(2)}(\cdot)$ represents the Hankel function of the second kind of order n; N_l denotes the truncation order of the l-th expansion, and k_1 is the wavenumber in the scatterer. Since multipoles are singular at the origin, the expansion centers must lie outside the domain of interest [11]. Hence, similar to the scattered field in (1), the total field inside the dielectric object is approximated by a set of multipolar sources placed outside the object and k_1 interchanged by k_2.

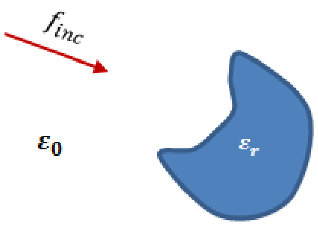


Fig. 1. Two dimensional configuration of the scattering problem.

In each domain, the corresponding multipoles satisfy the time harmonic Maxwell's equations. Accordingly, to determine the unknown coefficients in Eq. (1), one only needs to enforce the relevant boundary conditions. Note that multipole functions are independent of each other [25], but they are not orthogonal. As a result, while the point matching method is a popular choice in the MMP, the number of matching points should be selected such that the resulting equation system is overdetermined [11]. The over-determination factor is usually considered to be about 2 or 3 [11, 21].

3- SUBSPACE FITTING

When solving a problem using the MMP, three sets of parameters should be initially set: expansion centers, expansion orders, and matching points. Among these parameters, the allocation of the expansion centers is the most important. Indeed, the two other parameter sets could be determined based on simple and efficient rules [7, 11]. However as we stated earlier, the search for the optimum set of parameters is not trivial and could be very computationally demanding [21]. In this section, based on results of a subspace fitting analysis, a new guideline is proposed and justified for the problem of allocation of multipoles' origins in the MMP.

Let us consider a set of N linearly independent plane wave incident fields. For each incident field, we have the scattered field f^{sct}, that is represented by M samples on the object's boundary. These samples are arranged in a matrix $\mathbf{F} \subset \mathbb{C}^{M\times N}$. Moreover, let $\mathbf{R} \subset \mathbb{R}^{2\times L}$ be a matrix whose columns are position vectors of the expansion centers. Subsequently, by applying the signal subspace fitting (SSF) [26, 7], the problem is formulated as the following least-squares minimization

$$R_{\text{opt}} = \arg\min_{\mathbf{R}} \|\mathbf{\Phi}_s - \mathbf{H}(\mathbf{R})\mathbf{A}\|_F, \quad (2)$$

where $\mathbf{A}$ is the vector of coefficients and $\mathbf{H}(\mathbf{R})$ denotes the discretization of multipole functions in Eq. (1). The Frobenius norm is also denoted by $\|\cdot\|_F$. Additionally, the matrix $\mathbf{\Phi}_s$ denotes the set of first r left singular vectors of $\mathbf{F}$, that span the signal subspace. The value of r is determined by locating the knee point in the logarithmic plot of the singular values of $\mathbf{F}$ [27]. As it is shown by Mosher et al. [28], the minimization problem in Eq. (2) is equivalent to the following maximization problem

$$R_{\text{opt}} = \arg\max_{\mathbf{R}} \left\|\mathbf{U}_H^{T}\mathbf{\Phi}_s\right\|_F, \quad (3)$$

where $\mathbf{U}_H$ represents the matrix of left singular vectors of $\mathbf{H}(\mathbf{R})$ that correspond to its non-zero singular values. Then, we can define an SSF pseudo-spectrum by

$$S(r) = \arccos\left(\frac{\|\boldsymbol{U}_H^T\boldsymbol{\Phi}_s\|_F}{\|\boldsymbol{\Phi}_s\|_F}\right). \quad (4)$$

As a matter of fact, this spectrum provides a global measure of the approximation error for a multipole expansion centered at the point $\mathbf{r}'$.

Now we consider the scattered field of various dielectric objects in free space. The specifications of these cases are listed in Table 1. For all the cases, plane wave incident fields are coming from 360 directions (uniformly spaced over 360°). To avoid committing the so-called inverse crime [29], the scattered fields are computed by using a finite element method (FEM). Since we are dealing with the scattered field, expansion centers must be inside the object. Since the scattered field is effectively band-limited [26], the expansion order is set to $N = \frac{r-1}{2}$. Subsequently, the resulting pseudo-spectrums are shown in Fig. 2. The results show that a multipole expansion better matches the signal subspace by moving farther from the boundary up to a critical point. This is not surprising since we expect the local behavior of multipoles to be reduced as their distance from the boundary increases.

Interestingly, the critical point belongs to a set of points with a special property. Let x be a point on the object's boundary, then we associate with x the set of all points inside the object whose closest point on the boundary is x. The critical point is then the associated point that is the farthest point from x. Indeed, this is the definition of the medial axis of the object [30]. The radius of the maximal disk (centered at the medial point and tangential to the boundary) is called the medial radius [31].

The medial axis of each object is also overlaid on its corresponding SSF spectrum in Fig. 2. From this figure, it is evident that in order to approximate the desired field at

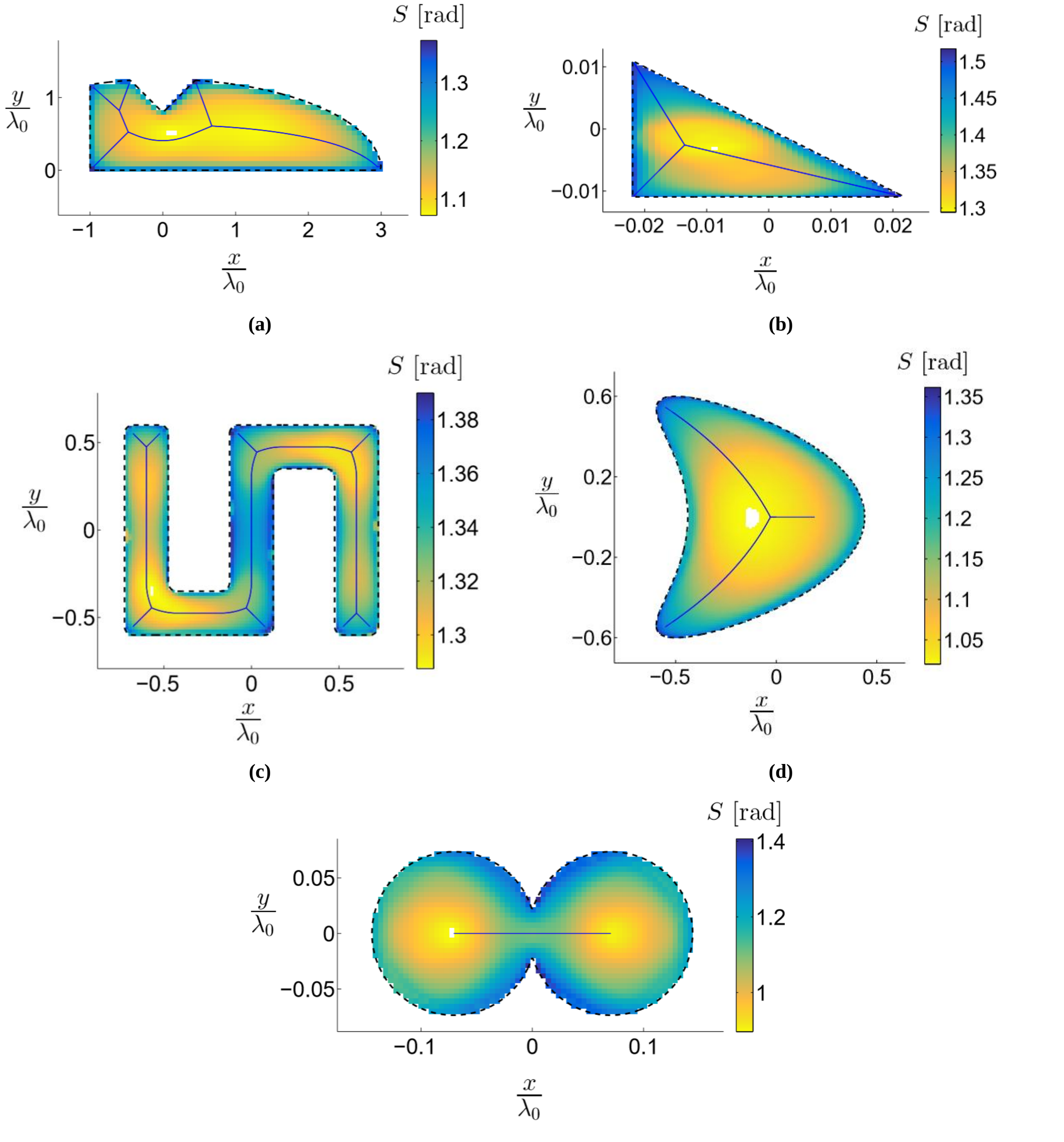


Fig. 2. The SSF spectrum (as defined by Eq. (4)) for various dielectric scatterers. The corresponding medial axis (solid) for each boundary (dashed) is overlaid on the SSF spectrum.

TABLE 1. DESCRIPTION OF THE TEST CASES IN FIG. 2.

Case ID	ε_r	Polarization	r
a	2	TM	68
b	$-7.34 - j0.23$	TE	13
c	2	TM	48
d	$6.80 - j1.14$	TM	33
e	$-1.16 - j0.30$	TE	23

each point on the boundary, the best location for a multipole expansion is almost on the medial axis. Note that the cases in Table 1 include objects with a wide range of sizes relative to the wavelength, different dielectric constants, and both the TE and TM polarizations. Consequently, the above observation is used to delineate the central idea of our expansion allocation guideline, that is, regarding the global approximation power of multipole expansions, the medial axis is the best location for an expansion.

Placing multipoles farther from the boundary increases their coverage domain [18]. As a result, the whole boundary is covered by a less number of multipoles when they are allocated on the medial axis. Consequently, by placing multipoles on the medial axis of the object the efficiency and accuracy of the MMP are improved at the same time.

The multipole allocation algorithm starts at the medial point corresponding to the maximum medial radius. Subsequently, those parts of the medial axis that lie inside the corresponding maximal disk are excluded from further processing. The algorithm repeats until processing all parts of the medial axis. Then, orders of selected multipoles are determined according to their corresponding medial radius, i.e. the larger the medial radius, the larger truncation order is assigned to the multipole expansion.

4- NUMERICAL SIMULATION

In this section two examples are presented to show the power of the MMP equipped with the allocation algorithm based on the proposed guideline. The first example is the full-wave simulation of a large object with the extent of about $50\lambda_0$ at $\lambda_0 = 500$ [nm]. As shown in Fig. 3, the object is an elliptic micro-lens. The major and minor semi-axes of the ellipse are 12 [um] and 6 [um], respectively. The relative permittivity of the object is $\varepsilon_r = 8.41$. A TM_z polarized incident field illuminates the object from the bottom.

Numerical simulation of such a large object is challenging since the number of unknowns and the computational burden of the solution may increase significantly with an improper set of multipole expansions. Additionally, MMP matrices are dense and it is important to select multipoles in such a way that it does not lead to a singular system matrix. Hence, the accuracy of the results will show the effectiveness of the proposed approach.

The distribution of multipoles along the medial axis (i.e. the line between the two foci) is shown in Fig. 3. Form Fig. 4 it is evident that the solution is converged for an expansion with a total order of about 3300. Subsequently, the distribution of the magnitude of the Poynting vector is compared with the FEM results in Fig. 5 which shows a very good agreement.

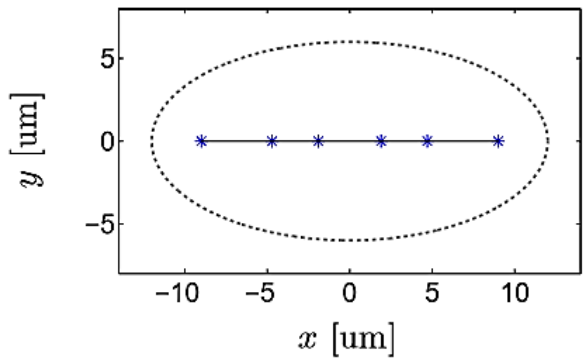


Fig. 3. The selected multipoles (markers) on the medial axis of the ellipse (solid) inside the object's boundary (dashed).

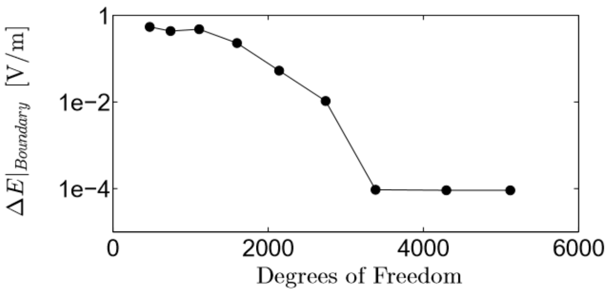
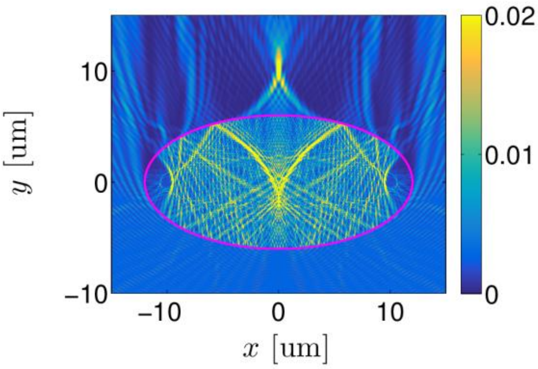
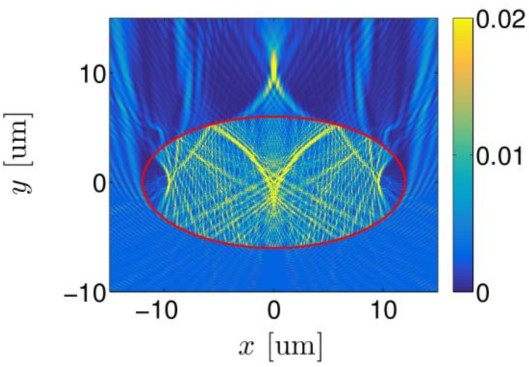


Fig. 4. Convergence of the MMP solution for the elliptic object.



(a)



(b)

Fig. 5. The distribution of the Poynting vector's magnitude (in [W/m^2]). a) MMP, b) FEM.

The next example is a triangle shaped silver nano-particle that its scattering properties is investigated in [7]. As shown in Fig. 6, the left and bottom sides of the triangle are 20 [nm] and 10 [nm], respectively. The relative permittivity of silver at the wavelength $\lambda_0 = 456$ [nm] is assumed to be $\varepsilon_r = -7.34 - j0.23$. The object is illuminated by a TE_z plane wave coming from the bottom left with its wavevector perpendicular to the triangle's hypotenuse. Like the previous example, the numerical modelling of the electromagnetic wave scattering by this particle is challenging since near the edges of the particle the electromagnetic fields are singular. In such a case, the accuracy of the solution depends on the density of multipoles near the edges. The distribution of the allocated multipoles along the medial axis of the triangle is shown in Fig. 6. As shown, close to the edge of the scatterer the density of multipoles is much higher than other parts of the object. As a result, we expect the MMP to be able to accurately model variations of the electromagnetic fields close to the edges.

The problem is solved with an average relative error of 0.0086% along the boundary and the convergence plot is depicted in Fig. 7. Similar to the results given by Moreno et al. [7], the magnitude of the electric field normalized to the incident field is depicted on a vertical line segment with $x = -5$ [nm] and $y \in (8,20)$ [nm] in Fig. 8. The MMP result is compared with the FEM one which shows a very good agreement. .The presented results show that the MMP equipped with the new allocation rule, could be used to readily solve the problem with a high accuracy.

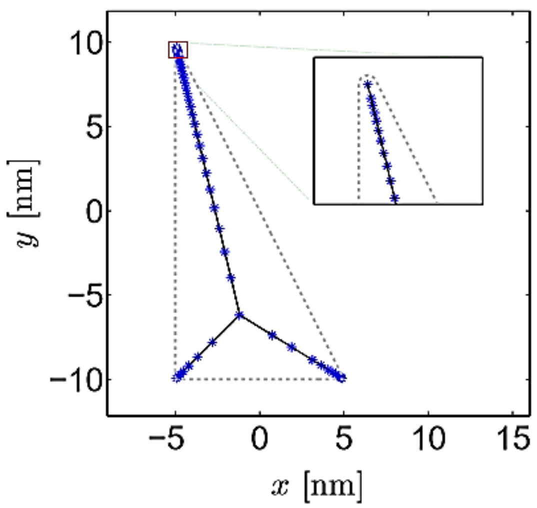


Fig. 6. The selected multipoles (markers) on the medial axis of the triangular scatterer (solid) inside the object's boundary (dashed). The inset plot shows the distribution of multipoles close to the top corner.

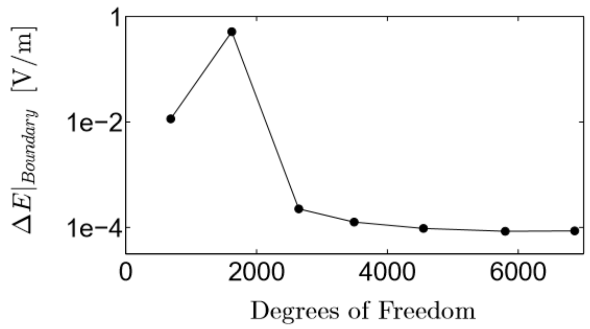


Fig. 7. Convergence of the MMP solution for the triangular object.

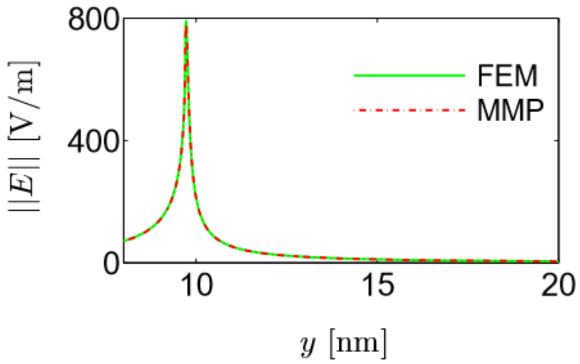


Fig. 8. The magnitude of the electric field computed by the MMP (dash dotted) compared to the FEM solution (solid).

5- CONCLUSIONS

The problem of multipole allocation in the MMP method is addressed by proposing a new allocation rule. The new guideline is justified using subspace fitting analysis which makes it different form present heuristic rules of thumb. The results show that placing multipoles on the medial axis of the scatterer increases their effectiveness which means a smaller number of multipole expansions and more accurate results. Two numerical examples are presented to show the validity and accuracy of the results by using the new rule for the allocation of multipole sources of the scattered field.

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