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# Analyzing Generalized Matching Point Technique (GMT) in Order to study Electromagnetic Interaction with Nanoparicles

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ABSTRACT

In this paper, semi-analytical generalized matching point technique (GMT) is investigated in order to study the interaction between electromagnetic wave and nanostructures. GMT code is developed in MATLAB software. To validate the code, both analytical Mie theory and semi-analytical GMT method are applied simultaneously for simulating scattered field from dielectric cylinder and a gold nanowire in vacuum which are both illuminated by a TM polarized plane wave. It can be seen that the agreement between both techniques is excellent. It is turned out that nanojet in dielectric micro-cylinder and localized surface plasmon (LSP) in gold nanowire are formed which both Mie and GMT techniques predict the same result.



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## INTRODUCTION

Analyzing the interaction of electromagnetic waves with nano cylindrical and spherical particles by using different numerical techniques has been the subject of intense investigation and research, recently. Employing an optimum method by regarding the condition governing these sorts of problems is a really crucial subject. Generalized Mie theory has been introduced as a regular analytical solution for studying light scattering with spherical and cylindrical particles [2,3]. Since generalized Mie theory is just capable of computing scattered field from a single sphere or a single cylinder, so for simulating more complex problems and also for achieving more realistic results, various numerical methods are being applied. For instance, finite differential time domain (FDTD) and finite element (FEM) techniques can be mentioned. FDTD method is a high-resolution code which is performed in time domain. Time consuming and instability are regarded as the most important disadvantages of this numerical technique. Moreover, it is required to mesh the simulation space as fine as possible in order to obtain reliable results that need really high computation resources. Thus, employing boundary methods in frequency domain may be more convenient, since only interfaces need to be descritized. The generalized matching point technique (GMT) is a good semi-analytical candidate for satisfying all computational requirements. GMT is a technique which works in frequency domain and as it is claimed to be semi-analytical solution so it possesses a very high accuracy and precision that is valuable when nanostructures are explored. The other strong feature which makes this method unique is that GMT is fast in manipulating heavy computing. It should be pointed out that the optimum location of multipoles is explored by trial and error. Hence, arranging them in a way that the residual is minimized is an extremely difficult task.

Photonic nanojets appear on the shadow side of the illuminated dielectric particle [11]. These particles create narrow and high intensity beams undergo the diffraction limit in the near field of the particle surface. With advent of achieving the undergo diffraction limit knowledge, lots of applications have been turned out including scanning near-field optical microscopy (SNOM) [12], high resolution lithography, advanced optical (and magnetic) data storage schemes, sensing and metrology, optical trapping, nano-patterning and immersion lens microscopy, Raman spectroscopy and for fluorescence imaging of living cells such as single molecules [4,6]. On the other hand, metallic nanostructures have broad application in nanoptic due to surface plasmon and localized surface plasmon phenomena [7]. Hence, with respect to wide practical domain, studying and investigating an optimum method for modeling these sorts of structures is absolutely a vital task [11].

In this paper, we present the generalized matching point technique initially. Afterwards, this numerical method is adapted for simulating the scattered field outside a dielectric micro-cylinder and a gold nanowire, as

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well. Finally, to validate the developed GMT code, the simulation results are compared with analytical Mie theory and it would be shown that both techniques reach to the same results.

*GMT theory:*

The generalized matching point technique was developed in Swiss Federal Institute of Technology by Hafner in 1980. The GMT is a semi-analytic boundary method working in the frequency domain for calculating electromagnetic fields via solving Maxwell equations in linear, isotropic and homogenous media and provide highly accurate results. The GMT has originated from the analytical Mie theory, circular harmonic analysis and point matching. Hence, the GMT method is claimed to be semi-analytical because the approximation to the actual field analytically satisfies the Maxwell differential equations, while the algebraic boundary conditions are approximately fulfilled at matching points.[7]

The GMT technique is based on this reality which every arbitrary electromagnetic field in the medium can be expanded by harmonic basis functions that are defined as orthonormal set. It should be concerned that harmonic basis functions must satisfy 2D Helmholtz equation, essentially.

*Basis functions and field expansions:*

A peculiarity of GMT is the high degree of freedom in selection of harmonic basis functions, in particular the multipolar functions. Modeling an electrodynamics problem with multipolar sources requires physical concepts. As it was mentioned before, fields can be simulated as a superposition one or more multipolar sources everywhere. If the point, that the fields are to be calculated there, is located inside the domain where the origins of multipoles have been placed, to prevent singularity, Bessel functions would be employed. Likewise, if the fields computing point is located outside the region of multipole origins, Henkel functions would be substituted instead of multipolar functions, since Henkel functions are singular in the origin whereas do not vanish at infinity. In the multiple multipole program (MMP), which is a special kind of GMT method, Henkel functions are adapted for field expansion [8]. Therefore, according to figure (1), in order to model the electromagnetic field in domain $D_i$ the origins of multipolar functions have to be located in region $D_i$ and similarly, to model the fields in domain $D_j$ multipolar function origins have to be placed in region $D_i$.

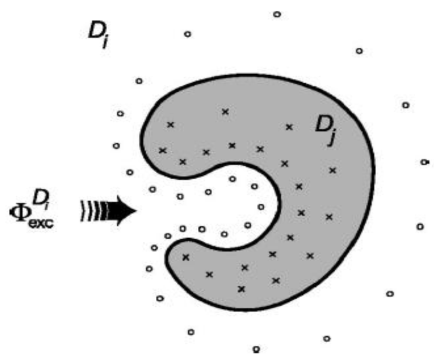


**Fig. 1:** Multipole expansion distribution. For modeling the electromagnetic field in domain $D_i$ the origins of multipolar functions have to be located in region $D_i$ and similarly, to model the fields in domain $D_j$ multipolar function origins have to be placed in region $D_i$ . The o's and ×'s denote the origins of multipole in domain $D_i$ and $D_j$ , respectively.

In GMT method, to model 2D electrodynamics problems such as problems with cylindrical structure (i.e. structures that are invariant along one axis (cylinder axis)) the knowledge of longitudinal components of the electric and magnetic fields $\{E_z^{D_i,D_j}, H_z^{D_i,D_j}\}$, is sufficient to derive the transverse electric field $E_T^{D_i,D_j}$ and magnetic field $H_T^{D_i,D_j}$ in both domains $D_i$ and $D_j$. Therefore, according to figure (1), when an electromagnetic emission interacts with a particle $(\varphi_{exc}^{D_i})$, the longitudinal components of both $E_z^{D_i,D_j}$ and $H_z^{D_i,D_j}$ are formulated in a following form in a transverse plane:

$$E_z^{D_i,D_j} = \sum_{l=1}^{L}\sum_{n=0}^{N_l}\left[A_{n_l}^{E} Z_n\left(K_T^{D_i,D_j} r_l\right)\cos(n\varphi_l) + B_{n_l}^{E} Z_n\left(K_T^{D_i,D_j} r_l\right)\sin(n\varphi_l)\right] \quad (1)$$

$$H_z^{D_i,D_j} = \sum_{l=1}^{L}\sum_{n=0}^{N_l}\left[A_{n_l}^{H} Z_n\left(K_T^{D_i,D_j} r_l\right)\cos(n\varphi_l) + B_{n_l}^{H} Z_n\left(K_T^{D_i,D_j} r_l\right)\sin(n\varphi_l)\right] \quad (2)$$

$$K_T^{D_i,D_j} = \sqrt{\varepsilon^{D_i,D_j}\mu^{D_i,D_j}\omega^2 - \gamma^2} = \sqrt{\varepsilon^{D_i,D_j}\mu^{D_i,D_j}\omega^2 - k_z^2} \quad (3)$$

s where $l$ denotes the number of multipoles, n is the order of multipole, L and $N_l$ represent maximum number and order of essential multipoles, respectively, $(r_l, \varphi_l)$ represent the polar coordinate of observing point from the $l$th multipole view and $Z_n(K_T^{D_i} r_l)$ is a determined cylindrical function, in which depending on multipole distribution, can be substituted by Bessel or Henkel functions. Thus, if Henkel functions $H_n$ are used as cylindrical functions, the expansion would be called singular multipole since Henkel is singular in the origin, so it is appropriate to be adapted for describing the scattered field. .$A_{n_l}^E$ , $A_{n_l}^H$ , $B_{n_l}^E$ , and $B_{n_l}^H$ are expansion coefficient which have to be determined. In equation (3), $K_T^{D_i}$ is the transverse wave number, $\varepsilon^{D_i}$ and $\mu^{D_i}$ denote permeability and permittivity coefficient in domain $D_i$ , respectively, and $\nabla_T$ represents the gradient in XY plane. When both $E_z^{D_i,D_j}$ and $H_z^{D_i,D_j}$ satisfy the 2D Helmholtz equation in $D_i$:

$$\left[\nabla_T + \left(K_T^{D_i,D_j}\right)^2\right]\begin{pmatrix} E_z^{D_i,D_j} \\ H_z^{D_i,D_j} \end{pmatrix} = 0 \tag{4}$$

then, the transverse components of electric and magnetic fields fulfill the differential Maxwell equations in $D_i$:and are derived in the following form:

$$E_T^{D_i,D_j}(r) = \frac{i}{\left(K_T^{D_i,D_j}\right)^2}\left[k_z \nabla_T E_z^{D_i,D_j}(r) - \omega\, \mu^{D_i,D_j}(\widehat{e_z} \times \nabla_T) H_z^{D_i,D_j}\right] \tag{5}$$

$$H_T^{D_i,D_j}(r) = \frac{i}{\left(K_T^{D_i,D_j}\right)^2}\left[k_z \nabla_T H_z^{D_i,D_j}(r) + \omega \varepsilon^{D_i,D_j}(\widehat{e_z} \times \nabla_T) E_z^{D_i,D_j}\right] \tag{6}$$

where $\widehat{e_z}$ is a unit vector along the Z axis.

*Boundary conditions:*

Therefore, according to figure (1) and with respect to the presented expansions, the total field in domain $D_i$ is given by

$$\varphi_{app}^{D_i} = \varphi_{exc}^{D_i} + \varphi_{sca}^{D_i} \tag{7}$$

where $\varphi_{app}^{D_i}$ denotes the approximation to the actual field, term $\varphi_{exc}^{D_i}$ represents determined exciting field ,and $\varphi_{sca}^{D_i}$ is unknown scattered electromagnetic field in the corresponding domain and is replaced by proper expansions given in equations (1), (2), (5), and (6). To determine the unknown coefficients based on media properties and also polarization of incident radiation, the appropriate weighted boundary conditions are imposed on the set of collocation points along the interface. So that, according to figure (2), the boundary of particle is partitioned in some segments. Within GMT method, to impose boundary condition, a generalized point matching (GPM) technique is utilized in order to minimize the weighted residual of electromagnetic field continuity within a finite number of matching points on boundary of object between homogenous domains. Thus, applying the proper continuity conditions on tangential and transverse components of electromagnetic field along all of the matching points may lead to a matrix equation of type

$$\sum_\beta A_{\alpha\beta} F_\beta = G_\alpha \tag{8}$$

where, $A_{\alpha\beta}$ is a rectangular matrix, the vector $F_\beta$ includes the unknown coefficients and the vector $G_\alpha$ stems for excitation. In order to reduce the numerical errors and also for more continuity on interface, the technique,

GMT method works with more equations (usually 2 or 3 times) than unknowns which is leading to an overdetermined system, and would be solved numerically. Eventually, after determining unknown coefficients, it is possible to compute field and also all other physical quantities such as pointing vector at every arbitrary point.

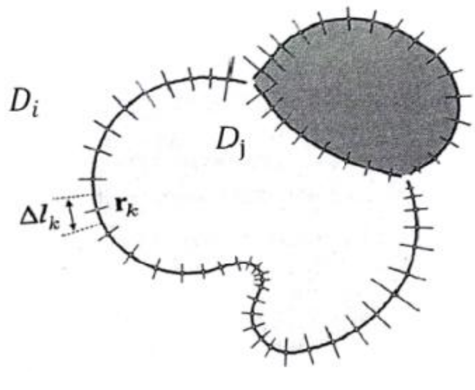


**Fig. 3:** Partitioning the interface between domains $D_i$ and $D_j$ , to impose boundary conditions in GMT method

*2D GMT simulation:*

In this paper, we report on the manipulation of GMT method for simulating scattered field from a dielectric micro-cylinder and also a gold nanowire which are illuminated by a plane harmonic wave such a way that the direction of the propagation is perpendicular to the cylindrical axis and it has TM polarization (i.e., the waves in which their components $H_z$ and $E_T$ are not zero). Afterwards, we compare the computational results with analytical Mie solution, as well. As the first attempt, we have to determine the optimum position of multipoles due to the medium condition and also the geometry of relevant structure. Suppose a micro-cylinder in a way that its axis is along the Z axis, as a result the symmetry axis would be Z axis. As it is shown in figure (3), the problem possesses symmetry. So, just one multipole is sufficient for modeling scattered field and similarly one for simulating internal field. The optimum location of both multipoles is in the center of circle (cylinder cross section).

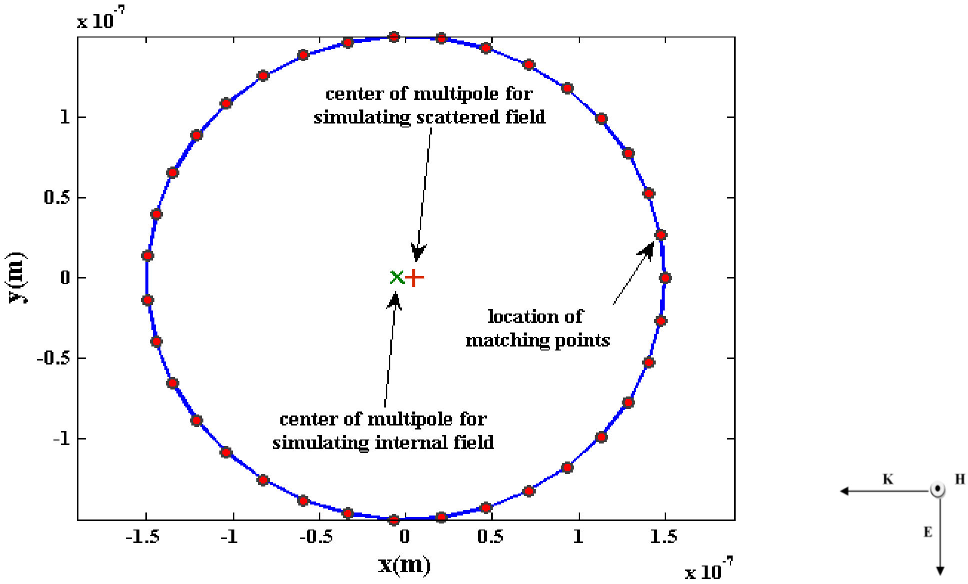


**Fig. 3:** 2D GMT simulation space geometry: the ●'s denotes the location of matching points on cylinder interface and ×'s and +'s represent multipole origins to model internal and scattered fields, respectively. The properties of plane wave are indicated at the right side. Cylinder axis is along Z direction.

Since the origin of multipole modeling the internal field is inside the micro-cylinder, so, as it was mentioned before, we employ Bessel function as cylindrical functions in the expansions represented for electromagnetic field to avoid singularity in the center. Likewise, as the multipole origin, simulating scattered fields is located outside the scattering region, so that, it is reasonable to apply Henkel function in the corresponding expansion because Henkel functions are finite at infinity. Due to the polarization of incident wave (TM polarization), it is just sufficient to impose tangential boundary condition on electric and magnetic field components along all collocation points in order to determine the unknown coefficients. It is worth mentioning that if the numbers of multipolar expansion terms applied for modeling scattered and internal fields are less than an optimum value, so the convergence may not be achieved and the simulation results would be far from reality.

## RESULTS AND DISCUSSIONS

In this framework, to study the scattering problem we have developed the GMT code in MATLAB. A dielectric cylinder with radius R=2μm is illuminated by a unit amplitude plane wave with operating wavelength $\lambda = 400nm$ and also TM polarization. The refractive index of this micro-cylinder is n=1.45 and the background medium is vacuum ($n_{out} = 1$). In order to validate the developed code, we compare the simulation data of scattered field intensity with analytical Mie theory as it is depicted in figure (4).

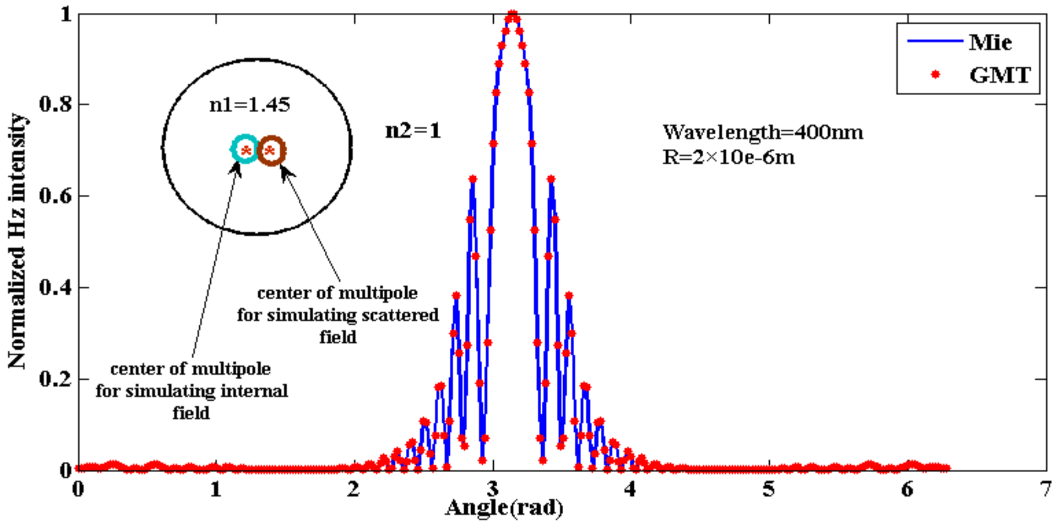


**Fig. (4):** A dielectric cylinder with radius R=2µm is illuminated by a unit amplitude plane wave with operating wavelength $\lambda = 400nm$ and also TM polarization. The background medium is vacuum.

In the figure (4) it can be seen that agreement between both techniques (including all the points particularly a maximum value of the scattered electric field intensity) is excellent and this indicates extreme convergence of GMT code. In this computation, we take the number of matching points on the boundary in a way that the outcome of imposing boundary conditions on them leads to numbers of equations which is two times more than numbers of unknown factors. It should be noted that the numbers of matching points cannot be chosen more than an optimum value due to the computation speed, on the other hand, as it was said before, the matching points numbers should not be selected too small such a way that the numbers of unknown terms become more than numbers of equations. In the corresponding dielectric micro-cylinder in order to calculate scattered field using GMT method, we placed just one multipole of order 46 in the center of the cylinder and the intensity of scattered $H_z$ is depicted as a function of angles between 0 to 2π at distance twice the radius (4µm) in figure (4).

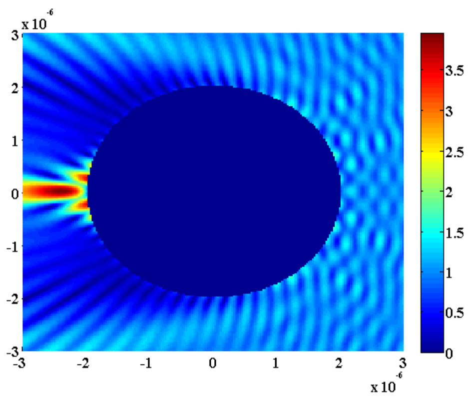

**Fig. 5:** 2D GMT simulation of scattered electric field intensity pattern from a dielectric cylinder with radius R=2µm is illuminated by a unit amplitude plane wave with operating wavelength $\lambda = 400nm$ and also TM polarization at distance twice the radius (4µm). The refractive index of this micro-cylinder is n=1.45 and the background medium is vacuum ($n_{out} = 1$).

Afterwards, we simulate the pattern of scattered electric field intensity at the distance twice the radius and with the same mentioned medium properties. The results are displayed in figure (5). As it is observed in figure (5), according to the represented concepts, nanonojet is provided just in the location where we expected, namely at the left end of micro-cylinder and exact in the direction of incident radiation. This is additional reason of GMT code validity and accuracy. Relative error graph of the respective computation is depicted in figure (6) and it is approximately in the order of $10^{-4}$ which indicates high precision of GMT technique.

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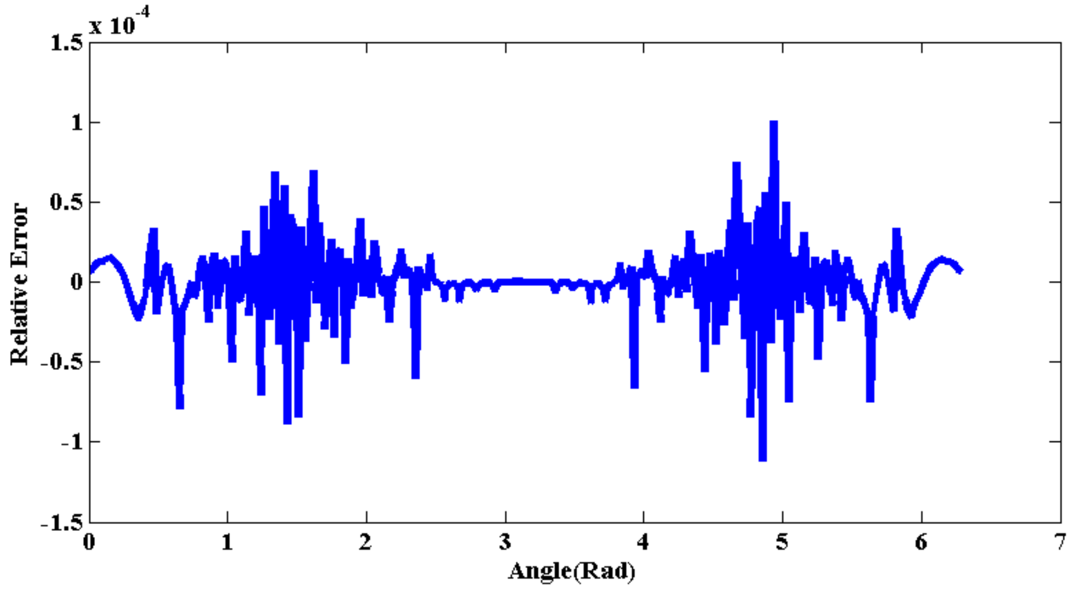


**Fig. 6:** Relative error graph in GMT method.

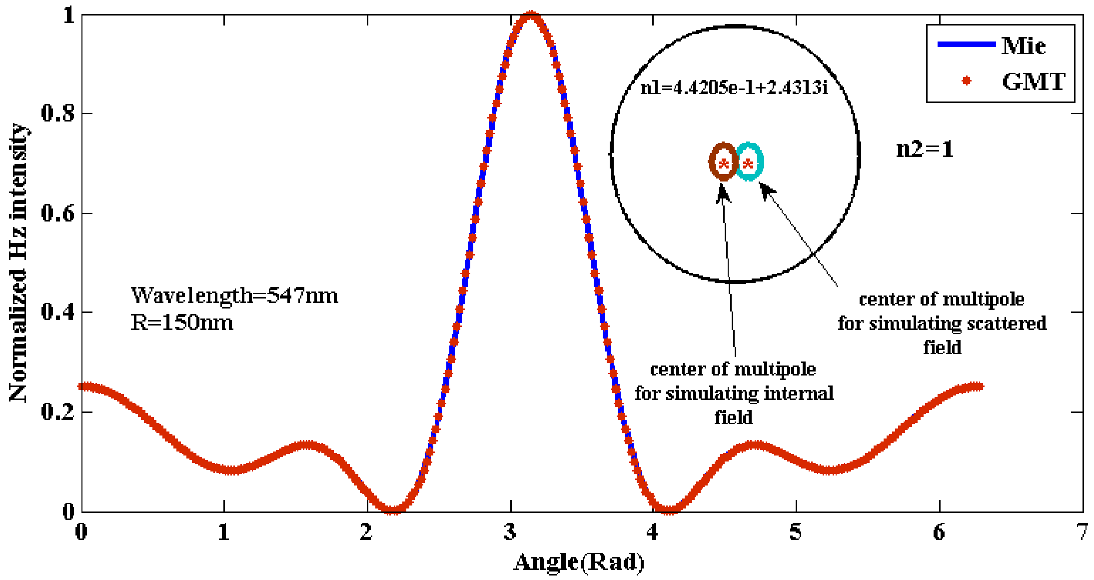


**Fig. 7:** 2D GMT simulation of the scattered magnetic field in Z direction from a gold nano-cylinder with radius R=150nm employing both Mie GMT methods. The background medium is vacuum ($n_{out} = 1$) and the refractive index of gold for incident wavelength (λ=547nm) is $n_{in} = .44205 + 2.4313i$

At the remainder of this paper, we investigate the simulation of interaction between electromagnetic field and gold nanowire which is important due to frequent application in optoelectric and nanoptic fields. The scattered magnetic field in Z direction from a gold nano-cylinder with radius R=150nm is presented. The background medium is vacuum ($n_{out} = 1$) and the refractive index of gold for incident wavelength (λ=547nm) is $n_{in} = .44205 + 2.4313i$.

The exciting electric field is contained in XY plane (i.e., TM polarization). In figure (7), the intensity of scattered $H_z$ is plotted as a function of angles between 0 to $2\pi$ at distance twice the radius (300nm) employing both Mie and GMT methods. Again due to the symmetry of the problem, the optimum place of multipole is in the center and just one multipole is enough. As it is observed in figure (7), the scattered $H_z$ intensity of gold nanowire under the mentioned physical properties, has a peak in angle $\pi$ radian. It is deduced that a plane wave with TM polarization and at operating wavelength λ=547nm excites localized surface plasmon (LSP) in the relevant gold nanowire. To prove this claim, we compute the scattering cross section of gold nanowire in the wavelength interval 200 to 1000nm using both Mie and GMT techniques. The results of calculations are indicated in figure (8). As we expected, scattering cross section is maximum in λ=547nm and $n_{in} = .44205 +$

2.4313i . It just demonstrates this reality that LSPR is formed in gold nanowire in the corresponding wavelength.

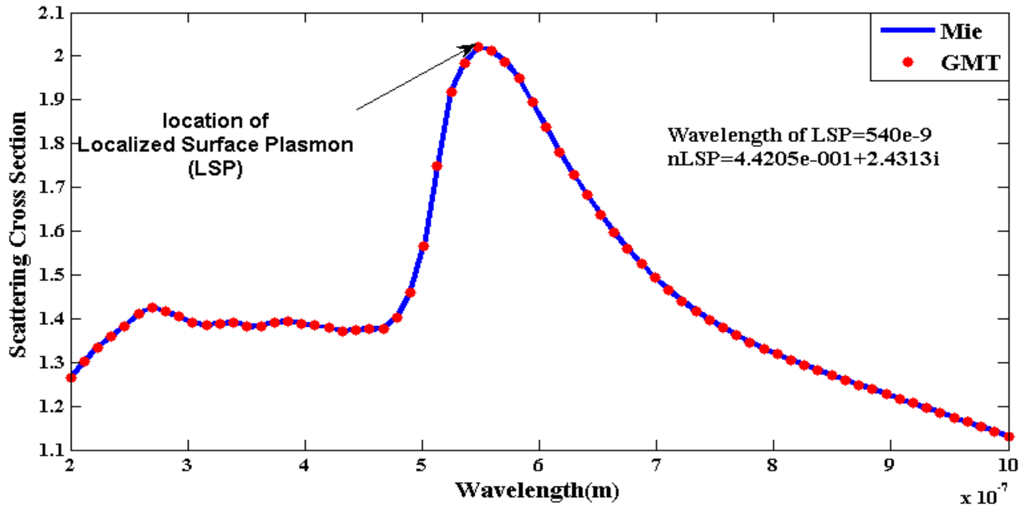


**Fig. 8:** Scattering cross section as a function of wavelength interval 200 to 1000nm using both Mie and GMT techniques. LSP is occurred in the wavelength λ=547nm.

*Conclusion:*

In this paper, we employed analytical Mie theory for modeling scattered field from a dielectric micro-cylinder and a gold nanowire in order to examine the semi-analytical GMT technique. By comparing Mie and GMT methods, we conclude that GMT technique as a semi-analytical method, compared with other numerical methods, possesses high accuracy and essential precision for modeling nanoptic and optoelectronic problems. Moreover, it is absolutely fast and has high convergence, as well. With regard to the performed simulations in this investigation, it is deduced that in GMT method the best and the most possible accurate place of multipole for modeling scattered field from a cylindrical structure is in the center of circle (cross section of cylinder) and also only one multipole is sufficient for this kinds of structures. In order to validate, both GMT code and Mie theory have been applied simultaneously, for simulating scattered field from a dielectric cylinder with refractive index $n_{in}$=1.45 and radius R=2μm in vacuum which is illuminated by a TM polarized plane wave with operating wavelength λ=400nm and the outcome agreed with Mie theory greatly. In this dielectric micro-cylinder scattered $H_z$ intensity was depicted as function of angles interval 0 to $2\pi$ at distance 2R and it was observed that $H_z$ intensity has its maximum value in π radian. Moreover, by plotting the pattern of electric field intensity in wavelength λ=400nm, nanojet – which its broad applications in nanoptic and optoelectronic fields was mentioned – was occurred. Likewise, same computation was held for modeling scattered field from a gold nanowire with refractive index $n_{in} = .44205 + 2.4313i$ and radius R=150nm in vacuum which is illuminated by a TM polarized plane wave with operating wavelength λ=547nm. Then, scattering cross section of the relevant nanowire was calculated and depicted as a function of wavelength interval 200nm to 1000nm. After analyzing and comparing scattered $H_z$ intensity graph and scattering cross section data, it was achieved that LSP was excited in the corresponding gold nanowire in wavelength λ=547nm while both of analytical Mie theory and semi-analytical GMT reached to the same result.

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