Regularization of jump points in applying the adaptive spatial resolution technique

Amin Khavasi and Khashayar Mehrany*
Department of Electrical Engineering, Sharif University of Technology, P.O. Box 11155-4363, Tehran, Iran

*E-mail: mehrany@sharif.edu

Abstract. The performance of the adaptive spatial resolution technique is improved by making the resolution function of the coordinate transformation as smooth as possible. To this end, the smoothness of the resolution function is probed and a quantitative criterion is proposed to make the jump points; which were conventionally equidistant from each other, regularized. The here-proposed regularization is applied to two different recent formulations and its effects on the overall convergence rate and on the presence of numerical artifacts in the analysis of highly conducting gratings are studied. Dielectric and metallic gratings at optical and microwave frequencies are considered and the helpfulness of the proposed technique is discussed.

Keywords: Diffraction and gratings, Diffraction theory, Fourier Modal Method.

1. Introduction

Although Fourier based methods are among the most popular rigorous techniques available for the analysis of diffraction gratings [1-3], there are still serious difficulties arising from the Gibb’s phenomenon and leading to extremely slowly convergent Floquet-Fourier series. The problem of slow convergence; becoming seriously troublesome in the analysis of metallic gratings illuminated by TM polarized waves, can be partly overcome by applying the Fourier factorization in representing the Fourier components of the continuous electromagnetic components [3]. The discontinuous and high-contrast grating profile; however, remains to be Fourier expanded, and can still incur extremely slow convergence rate. This is due to the fact that the spatial resolution within the modulated region is uniform in a Cartesian coordinate system and thus sharp discontinuities of the grating profile require keeping higher-order Fourier harmonics spoiling the overall convergence rate of the calculation. It is fortunately possible to increase the spatial resolution around the grating profile discontinuities by employing a new coordinate system and applying the adaptive spatial resolution (ASR) technique [4], wherewith the space is duly stretched and the overall convergence rate is accordingly accelerated. This is proved quite useful in the analysis of lamellar and trapezoidal gratings, where the Cartesian coordinate, $x$, is parametrically presented as a specific function of the transformed coordinate, $u$ [4-7]. This technique, however, is still problematic in the analysis of highly conducting gratings in which numerical artifacts appear because of violation of Li’s factorization rule [8-12]. There is therefore still room for further improvements. For instance, a simple modification that can substantially decrease the presence of numerical artifacts is recently made in the eigenvalue formulation of the ASR technique [13].
In this paper, the parametric transformation of the original Cartesian coordinate system used in applying the ASR technique is modified not by changing the eigenvalue formulation but by regularizing the jump points in the transformed space. This is done in such a fashion that the resolution function of the ASR becomes smoothened and thus the overall performance of the parametric coordinate transformation is considerably improved.

Two forms of the eigenvalue formulation, viz. the conventional [4] and the modified one [13], are examined by using two different approaches in choosing jump points in the transformed space, viz. the equidistant [7] and the here proposed regularization. The overall convergence rate and the presence of unwanted numerical artifacts are both investigated for different types of gratings. Interestingly, it is shown that employing the modified eigenvalue formulation cannot decrease the convergence rate in dielectric cases.

This paper is organized as follows: first, the parametric transformation of the coordinates is briefly reviewed and then the proposed strategy for regularizing the jump points in the transformed coordinate space is presented and heuristically justified. Before drawing the final conclusions, the overall convergence rate and the presence of numerical artifacts are investigated in sections 3 and 4.

2. Regularization of Jump Points

The most general one-dimensional lamellar grating is shown in figure.1, where the grating region with thickness \( d \) is characterized by a piecewise constant periodic permittivity profile \( \varepsilon(x) = \varepsilon(x + \Lambda_g) \), and separates two homogeneous media with refractive indices \( n_1 \) and \( n_3 \). This structure is illuminated by a linearly polarized monochromatic uniform plane wave with a vacuum wave-number \( k_0 = \frac{2\pi}{\lambda_0} \), having the incident angle of \( \theta \) with respect to the \( Oz \) axis.

In applying the ASR technique, the Cartesian coordinate \( x \) is parametrically presented as a function of a new coordinate \( u \), and the following change of variable is applied:

\[
x \rightarrow x(u) \Rightarrow \frac{\partial}{\partial x} \rightarrow \frac{1}{h(u)} \frac{\partial}{\partial u} \tag{1}
\]

\[
h(u) = \frac{dx}{du} \tag{2}
\]
where \( h(u) \) has been referred to as either the resolution function [5], or the scaling factor [4].

For TM polarization, the conventional formulation of eigenvalue problem in new coordinate \((u, y, z)\) reads as [4],

\[
\lambda^2_y H_y = \left[ \frac{1}{\varepsilon} \right]^{-1} \left[ \frac{1}{\varepsilon_0} \right]^{-1} K_x \left[ \frac{1}{\varepsilon} \right]^{-1} K_x - k_0^2 \left[ \frac{1}{\varepsilon} \right] H_y
\]

(3)

Here, \([f]\) denotes the Toeplitz matrix whose \((m, n)\) entry is the \((m-n)\)th Fourier coefficient of \(f(x)\); hereafter denoted by \(f_{m-n}\), \(I\) is the identity matrix and \(K_x\) stands for the diagonal matrix whose \(i\)th diagonal element is \(k_{xi} = k_0 n_i \sin \theta + 2 \pi i/\Lambda_G\). The eigenvalues, \(\lambda_y^2\), and eigenvectors, \(H_y\), make up the electromagnetic field distribution.

Equation (3) is recently modified and is written as [13]

\[
\lambda^2_y H_y = \left[ \frac{1}{\varepsilon} \right]^{-1} \left[ \frac{1}{\varepsilon_0} \right]^{-1} K_x \left[ \frac{1}{\varepsilon} \right]^{-1} K_x - k_0^2 I H_y
\]

(4)

This modification is shown to be successful in significantly decreasing numerical artifacts in the analysis of highly conducting gratings.

Regarding coordinate transformation, the following formula is conventionally used and proved to be efficient in substantially increasing the convergence rate of the problem [5, 7]:

\[
x_i(u) = a_1 + a_2 u + \frac{a_3}{2\pi} \sin \left( 2\pi \frac{u - x_{i-1}}{u_i - u_{i-1}} \right)
\]

(5-a)

The function \(x_i(u)\) stands for the mapping between two successive jump points \(l\) and \(l-1\). These jump points are denoted by \(x_l\) in the original coordinate system \((x, y, z)\) and by \(u_l\) in the new coordinate system \((u, y, z)\), and

\[
a_1 = \frac{x_l x_{l-1} - u_{l-1} x_l}{u_l - u_{l-1}}
\]

(5-b)

\[
a_2 = \frac{x_l - x_{l-1}}{u_l - u_{l-1}}
\]

(5-c)

\[
a_3 = G(u_l - u_{l-1}) - (x_l - x_{l-1})
\]

(5-d)

where \(G\) is a small enough numerical parameter that increases the spatial resolution near the discontinuities [5].

Although the jump points \(x_l\) in the original Cartesian coordinate system is already known, the transformed jump points \(u_l\) in the new coordinate system are not predetermined and are usually chosen to be equidistant from each other [7].

It can be easily seen that the convergence of equation (3) and (4) depends directly on the convergence rate of the Fourier series of the resolution function \(h(u)\). It is therefore logical to regularize the transformed jump points \(u_l\) by making the resolution function \(h(u)\) as smooth as possible. In this manner, the convergence speed of the Fourier series in the transformed space can be further increased. But the continuity of the resolution function \(h(u)\), and of its derivative \(h'(u)\) is already guaranteed if the
parametric representation of the coordinate transformation in equation (5) is applied. We are therefore left to focus on the second derivative of resolution function, \( h''(u) \), and propose its continuity as a concrete criterion to further smoothen the resolution function, and thus to regularize the jump points \( u_l \) in the transformed space. Despite sounding insubstantial, this regularization can significantly increase the overall convergence rate of the algorithm and decrease the bothersome presence of numerical artifacts in the analysis of highly conducting gratings.

Assuming \( G = 0 \) and after some algebraic manipulations, it can be shown that the continuity condition of \( h''(u) \) across the transformed jump points \( u_l \) necessitates the holding of the following equation:

\[
\Delta u_k = \frac{3\sqrt{\Delta x_k}}{3\sqrt{\sum_l \Delta x_l}} \tag{5}
\]

where \( \Delta u_k = u_k - u_{k-1} \), and \( \Delta x_k = x_k - x_{k-1} \).

3. Convergence Investigation

We apply the Fourier modal method with stable implementation of ASR [14]. In this approach, the eigenvalue problem has to be solved in every three regions: grating region and two homogenous regions. It should be however noticed that once the problem is solved in one of the homogenous regions the solution of the other can be easily extracted [15].

In accordance with the formulation given in the previous section, four different strategies can be followed:

1- Using (3), the conventional formulation of ASR, and applying equidistant method for choosing jump points in the new coordinate. This type of implementation is hereafter referred to as the conventional adaptive spatial resolution with equidistant jump points (C-ASR-EDJP).

2- Using (3), the conventional formulation of ASR, and applying the proposed regularization method for choosing jump points in the new coordinate. This type of implementation is hereafter referred to as the conventional adaptive spatial resolution with regularized jump points (C-ASR-RJP).

3- Using (4), the modified formulation of ASR, and applying equidistant method for choosing jump points in the new coordinate. This type of implementation is hereafter referred to as the modified adaptive spatial resolution with equidistant jump points (M-ASR-EDJP).

4- Using (4), the modified formulation of ASR, and applying the proposed regularization method for choosing jump points in the new coordinate. This type of implementation is hereafter referred to as the modified adaptive spatial resolution with equidistant jump points (M-ASR-RJP).

To compare the convergence performance of these four strategies in implementation of the ASR technique, we consider a simple lamellar grating, which has two regions \( x_0 = 0 < x < x_1 \) filled with a homogeneous material whose permittivity is \( \varepsilon_{21} = 1 \), and \( x_1 < x < x_2 = \Lambda_G \) filled with a homogenous material whose permittivity is \( \varepsilon_{22} \). In our case, \( x_1 = 0.05\Lambda_G \) (i.e. 95 percent of the grating is filled by \( \varepsilon_{22} \)). In accordance with figure 1, the other parameters of the structure are \( d = \Lambda_G = 1 \), \( \lambda = 1.4\Lambda_G \), \( \theta = 0 \) and \( \varepsilon_1 = \varepsilon_3 = 1 \). The reflected power from this structure, when it is illuminated by a TM polarized wave, has been plotted versus the number of retained space harmonics in figures 2 to 4, for \( \varepsilon_{22} = (0.0187 - j3.8069)^2 \) (the permittivity of a good metal in optical frequencies), \( \varepsilon_{22} = 1 - j10^7 \) (the permittivity of a good metal in microwave frequencies) and \( \varepsilon_{22} = 11.56 \) (the permittivity of a dielectric), respectively. In these figures, the results are obtained by employing all possible implementations.
discussed in the previous section, i.e. M-ASR-EDJP (dashed line), C-ASR-EDJP (dotted line), M-ASR-RJP (solid line), C-ASR-RJP (dashed-dotted line).

Figure 2. The reflected power of a good metallic grating at optical frequencies versus the number of retained space harmonics: M-ASR-EDJP (dashed line), C-ASR-EDJP (dotted line), M-ASR-RJP (solid line), C-ASR-RJP (dashed-dotted line).

Figure 3. The reflected power of a good metallic grating at microwave frequencies versus the number of retained space harmonics: M-ASR-EDJP (dashed line), C-ASR-EDJP (dotted line), M-ASR-RJP (solid line), C-ASR-RJP (dashed-dotted line).
If jump points are equidistant, the convergence rates of the two formulations (3) and (4) depend on type of the grating. For our working example, the convergence rate of the modified formulation is better for the metallic grating at optical frequencies (figure 2). For the dielectric grating; on the other hand, the conventional formulation is the winner (figure 4). Interestingly, the performance of both formulations is almost the same for the metallic grating at microwave frequencies (figure 3). Although the performance of the modified and conventional formulations given in equations (3) and (4) depend on the permittivity coefficients and the frequency regime, the proposed regularization is always beneficial, no matter to what type and which formulation it is applied.

The foremost reason for the beneficence of applying the proposed regularization is that the convergence rate of both modified and conventional formulations in homogenous regions is solely determined by the convergence rate of the resolution function’s Fourier series, which is here augmented by making it smoother. It is worth noticing that there is no reason to believe that increasing the convergence rate of the resolution function’s Fourier series can considerably increase the overall convergence of equations (3) and (4) in the grating region. It is thus no surprise that the observed improvement for metallic gratings at microwave frequencies is quite marginal because the overall convergence rate is in this case decreed by the convergence rate in the grating region and not the neighboring homogeneous media. This is due to the fact that the discontinuity of the permittivity profile in the grating region in such cases is so harsh that even the ASR technique is not capable of augmenting its convergence in the Fourier domain.

4. Highly conducting gratings

For highly conducting gratings in optical frequencies, the metallic region has negative permittivity while the dielectric region has positive one. The simultaneous presence of negative and positive values in the permittivity profile leads to the violation of conditions necessary for the validity of Fourier factorization rules [11]. Consequently, numerical artifacts appear in the analysis of highly conducting
gratings with Fourier based methods. It is already shown that increasing the number of harmonics retained in truncation can diminish this problem [11]. It is also shown that applying the ASR technique would be a considerable further help [13]. Nevertheless, an important question remaining to be answered is which of the four possible strategies listed in the previous section is more effective in decreasing numerical artifacts.

To address this question, a simple binary grating is investigated. The metallic region between \( x_0 = 0 < x < x_1 = f \) is made of a lossless metal whose permittivity at the free space wavelength \( \lambda_0 = 632.8 \) nm is assumed to be \( \varepsilon_m = (-10j)^2 \). Region 3 is a homogeneous metallic region with the same permittivity and region 1 is free space. This structure is illuminated by a TM polarized plane wave whose angle of incidence is \( \theta = 30^\circ \). The grating periodicity and thickness are \( \Lambda_G = d = 500 \) nm and 31 space harmonics is retained in this calculation. The minus first reflected order is plotted in figure. 5 (a), (b), (c) and (d) as a function of \( \tau = 1 - f \), by using C-ASR-EDJP, C-ASR-RJP, M-ASR-EDJP and M-ASR-RJP, respectively. These figures clearly demonstrate the superiority of the modified formulations in decreasing the presence of numerical artifacts. They also show that the proposed regularization is justifiable when it is applied to the conventional formulation.

Figure 5. Diffraction efficiency of the minus first reflected order versus fill factor of a highly conducting binary grating: (a) C-ASR-EDJP, (b) C-ASR-RJP, (c) M-ASR-EDJP and (d) M-ASR-RJP.
5. Conclusion

The position of the transformed jump points, $u_\delta$, in applying the ASR technique has been thus far rather arbitrary. In this paper, the smoothness of the resolution function is introduced as a criterion to regularize the transformed jump points. The proposed regularization is then applied to two different eigenvalue formulations (the conventional in [4] and the modified in [13]) and its performance is then compared against that of the either of these two formulations employed with no regularization. Dielectric and metallic gratings, the latter at both microwave and optical frequencies, are studied to see which of the four possible strategies in applying the ASR technique is justifiable. It is shown that while applying the regularization is quite useful in augmenting the convergence rate in the analysis of dielectric gratings, it makes no big difference if it is applied to metallic ones. It can however decrease the presence of numerical artifacts in the analysis of highly conducting gratings particularly if it is applied to the conventional formula in [4]. As a matter of fact, the use of regularized jump points in the conventional formula is shown to be as effective as using the modified formula.

References: