Least-squares method for the diffraction problem of strip gratings

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Abstract. In this paper, we focus on the diffraction problem of periodic strip gratings. A least-squares non-polynomial finite element method is proposed for this problem. Firstly, the computational domain is decomposed. Secondly, a local approximation space is defined by using non-polynomial functions in every subdomain. Then the least-squares finite element method is derived. Finally, numerical results are reported to show the effectiveness and convergence of the least-squares non-polynomial finite element method.

1. Introduction
The scattering theory of periodic structures has a wide variety of applications in the design of micro and nanoscale optical components, spectral analysis, etc. The periodic structure is also called diffraction gratings in optics [1]. There are many numerical methods for this diffraction problem, such as integral equation method [2], finite element method (FEM) [3-4], spectral method [5]. When the traditional FEM is used to solve the Helmholtz equation problems, 6-10 nodes are needed in a wavelength range, which causes the pollution effect. Especially when the wave number is large, the traditional finite element method is not practical [6]. In recent years, a least-squares non-polynomial finite element method is appropriate to normal diffraction gratings and the cases with large wave number. Therefore, this paper attempts to use a least-squares non-polynomial FEM to solve diffraction problem of strip gratings. The computational domain is decomposed and in every domain, we choose the appropriate bases to obtain the fast convergence. In addition, the method uses expansions by local polar coordinate, which can deal with the singularity at the end of the slit.

2. Diffraction problem of strip gratings
In this section, we introduce some notations to describe the diffraction problem of strip gratings with period $d$, see Figure 1. Assume that the length of the perfect conductive material strips is $s_1$, and the length of each slit is $s_2$, where $s_1 = s_2$. In one period, we denote the strips by $\Gamma_a$ and $\Gamma_c$, the slit between two strips by $\Gamma_b$, respectively:

$$\Gamma_a = \{(x_1,x_2) \in \mathbb{R}^2; \quad -\frac{d}{4} < x_1 < -\frac{d}{2}, x_2 = 0\},$$
$$\Gamma_b = \{(x_1,x_2) \in \mathbb{R}^2; \quad -\frac{d}{4} < x_1 < \frac{d}{4}, x_2 = 0\},$$
$$\Gamma_c = \{(x_1,x_2) \in \mathbb{R}^2; \quad \frac{d}{4} < x_1 < \frac{d}{2}, x_2 = 0\}.$$
Define
\[ \Omega = \left\{ (x_1, x_2) \in \mathbb{R}^2 : -\frac{d}{2} < x_1 < \frac{d}{2}, x_2 \in \mathbb{R} \right\}. \]

Suppose that the domain
\[ S = \Omega \setminus \left( \Gamma_a \cup \Gamma_c \right). \]

Figure 1. The diffraction problem of strip gratings

Assume that the plane wave \( u^i = e^{i(\alpha x_1 + \beta x_2)} \) is the incident wave upon the grating, where \( \alpha = k \sin \theta, \beta = k \cos \theta, k > 0 \) is the wave number, and \( \theta \in (-\pi/2, \pi/2) \) is the angle of incidence.

Denote the diffracted field by \( u_d \). Then the total field \( u \) is
\[ u = \left\{ \begin{array}{ll} u_i + u_d, & x_2 > 0, \\ u_d, & x_2 < 0, \end{array} \right. \]

and the diffraction problem of strip gratings reads as follows: when the incident field \( u_i \) is given, find the total field \( u \) such that
\[ \begin{cases} \Delta u + k^2 u = 0, & \text{in } S, \\ u = 0, & \text{on } \Gamma_a \cup \Gamma_c. \end{cases} \]

Considering the physical meaning of the equations above and the uniqueness of the solution, we need the following quasi-periodic condition, i.e.,
\[ u(-d/2, x_2) e^{i\alpha_0} = u(d/2, x_2). \]

Moreover, the diffracted field \( u_d \) is required to satisfy the bounded outgoing wave condition, which leads to the following Rayleigh expansion
\[ u(x_1, x_2) = u^i + \sum_{n=-\infty}^{\infty} a_n e^{i(\alpha_n + \beta_n) x_1 i \beta_n x_2}, \quad x_2 > 0, \]
\[ u(x_1, x_2) = \sum_{n=-\infty}^{\infty} b_n e^{i(\alpha_n + \beta_n) x_1 i \beta_n x_2}, \quad x_2 < 0, \]

where
\[ \alpha_n = 2\pi n / d, \quad \beta_n = \left\{ \begin{array}{ll} (k^2 - (\alpha_n + \alpha)^2)^{1/2}, & k^2 - (\alpha_n + \alpha)^2 \geq 0, \\ i((\alpha_n + \alpha)^2 - k^2)^{1/2}, & k^2 - (\alpha_n + \alpha)^2 < 0. \end{array} \right. \]

We further exclude resonances by assuming that \( k \neq |\alpha_n + \alpha| \) for all \( n \in \mathbb{Z} \).

3. Least-squares method

To construct numerical algorithm, the grating surface is assumed to be invariant in the \( z \) direction and periodic in the \( x \) direction, as shown in Figure 2. The endpoint of the strip grating is \( P_1 \) and \( P_2 \). Define the artificial boundaries
where \( n/2 \) the boundary of solution and the domains satisfies the Helmholtz equation and the zero boundary condition on subdomain in that period by \( n \) be a unit normal vector to the curve ,

In subdomains 1

Similarly, in domain 4

For a function \( v \in V \), define the matching error functional at the element interface as follows:

\[
V = \{ v \in L^2_{\text{loc}}(S); v|_{E_j} \in V_j, j = 1, 2, 3, 4 \}.
\]

\[
V_j = \left\{ \sum_{n=1}^{N_j} c_n^j J_{\nu}(kr) \sin \left( \frac{n \theta}{2} \right), c_n^j \in \mathbb{C} \right\},
\]

In domains 3

\[
V_j = \{ u_j(x_1, x_2) + \sum_{n=1}^{N_j} c_n^{(3)} e^{i(\alpha_n + \beta_n)\gamma_{1i} + \beta_n}, c_n^{(3)} \in \mathbb{C} \}.
\]

\[
\Gamma_h = \{(x_1, x_2) \in \mathbb{R}^2; -d/2 < x_1 < d/2, x_2 = h \},
\]

\[
\Gamma_h = \{(x_1, x_2) \in \mathbb{R}^2; -d/2 < x_1 < d/2, x_2 = -h \},
\]

\[
\Gamma_{h_\nu} = \{(x_1, x_2) \in \mathbb{R}^2; -d/2 < x_1 < d/2, x_2 = h \},
\]

\[
\Gamma_{h_\nu} = \{(x_1, x_2) \in \mathbb{R}^2; -d/2 < x_1 < d/2, x_2 = -h \}.
\]

The domain \( S \) is subdivided into four simply connected subdomains \( E_j, 1, 2, 3, 4 \). And we denote the boundary of \( E_j \) by \( \Gamma_j \). Suppose \( E_j \) satisfies the following conditions:

1. For \( j = 1, 2, E_j \) contains endpoint \( P_j \),
2. \( E_3 = U_h, E_4 = U_{h_\nu} \),
3. \( E_i \cap E_j = \emptyset \) for all \( i \neq j \),
4. \( \bigcup_j E_j = \bar{S} \),
5. Denote \( \Gamma_{ij} = \Gamma_j \cap \Gamma_j \), Shift the decomposition in \( S \) to its left neighbour period, denote the subdomain in that period by \( E'_j \) and the boundary of \( E'_j \) by \( \Gamma'_j \). Define \( \Gamma_{12}' = \Gamma_1 \cap \Gamma_2 \). Let \( n(x) \) be a unit normal vector to the curve \( \Gamma_{ij} \) or \( \Gamma'_{ij} \). Particularly, we define \( n(x) \) point \( E_2 \) to \( E_1 \), if \( x \) lies on \( \Gamma_{12} \).

In subdomains \( E_1 \) and \( E_2 \), we define the local polar coordinates. The origins are the endpoints \( P_1 \) and \( P_2 \). Therefore, using local polar coordinates in \( E_1 \) and \( E_2 \), the function \( v(r, \theta) \) which satisfies the Helmholtz equation and the zero boundary condition on \( \Gamma_n \) and \( \Gamma_c \),

\[
v(r, \theta) = \sum_{n=1}^{\infty} c_n^j J_{\nu}(kr) \sin \left( \frac{n \theta}{2} \right),
\]

where \( J_{\nu/2} \) represents the Bessel function of order \( \nu/2 \), \( c_n^j \in \mathbb{C} \). So in the subdomain \( E_j \), \( j = 1, 2 \), the total field \( u \) can be approximated by using the finite terms of the Fourier-Bessel expansion.

In every subdomain \( E_j, j = 1, 2 \), we define the local approximation space

\[
V_j = \left\{ \sum_{n=1}^{N_j} c_n^{(j)} J_{\nu}(kr) \sin \left( \frac{n \theta}{2} \right), c_n^{(j)} \in \mathbb{C} \right\},
\]

Since the functions in space \( V_j \) have the same singularity at \( P_j \) as the exact solution, the exact solution \( u \) can be better approximated.

In domain \( E_1 \), by the Rayleigh expansion, we define the approximation space

\[
V_1 = \{ u(x_1, x_2) + \sum_{n=1}^{N_1} c_n^{(1)} e^{i(\alpha_n + \beta_n)\gamma_{1i} + \beta_n}, c_n^{(1)} \in \mathbb{C} \}.
\]

Similarly, in domain \( E_4 \), we define the approximation space

\[
V_4 = \left\{ \sum_{n=N_4}^{N_4} c_n^{(4)} e^{i(\alpha_n + \beta_n)\gamma_{1i} + \beta_n}, c_n^{(4)} \in \mathbb{C} \right\}.
\]

Combining the spaces above, we can define the trial space \( V \) as follows:

\[
V = \{ v \in L^2_{\text{loc}}(S); v|_{E_j} \in V_j, j = 1, 2, 3, 4 \}.
\]
\[ J(v) = \sum_{\gamma \in j} \int_{\Gamma_{\gamma,j}} \left( k^2 \left[ [v]\right]^2 + \left[ [\partial v / \partial n]\right]^2 \right) ds + \int_{\Gamma_{\gamma,t}} \left( k^2 \left[ [v]\right]^2 + \left[ [\partial v / \partial n]\right]^2 \right) ds, \]

where \([v]\) represents the jump of function \(v\) at the interface of the different regions

\[
[v] = \left\{ \begin{array}{ll}
\lim_{\varepsilon \to 0^+} (v(x + \varepsilon n(x)) - v(x - \varepsilon n(x))), & x = (x, y) \in \Gamma_{i,j}, \\
\lim_{\varepsilon \to 0^-} (v(x + \varepsilon n(x)) - e^{i\alpha \varepsilon} v(x - \varepsilon n(x))), & x = (0, y) \in \Gamma_{i,2}, \bar{x} = (d, y).
\end{array} \right.
\]

The jump of \(\partial v / \partial n\) is defined in the same way, and denoted by \(\left[ \partial v / \partial n \right]\). Then our least-squares finite element solution \(u_N\) is defined as the solution of the following least-squares problem:

\[ u_N = \arg \min_{v \in W} J(v). \]

We can obtain the following error estimate.

**Theorem.** Assume that \(k^2 \neq \left( \alpha_n + \alpha \right)^2\) for all \(n \in \mathbb{N}\), and \(u_N\) is the solutions of the least-squares problem, then there exists a constant \(C > 0\) such that

\[ \left\| u - u_N \right\|_{H^{-1/2}} \leq CJ(u_N)^{1/2}. \]

The proof of Theorem 1 is similar to the proof of Theorem 3.1 in [7]. This theorem shows that for arbitrary non-resonant wave numbers \(k, J(u_N)^{1/2}\), controls the internal error of the solution. In Figure 3, if \(J(u_N)^{1/2}\) is large, the error of the solution is large, and the number of bases needs to be increased to obtain a more accurate solution.

**Example 1.** Take the grating period as \(d = 2\), the length of perfect conductive material strips \(s_1 = 1\) and the length of the slit \(s_2 = 1\). The incident wave is plane wave with the incident angle \(\theta = \pi / 4\). In figure 3, we show the convergence result of functional \(J(u_N)^{1/2}\). We can know that as the number of bases \(N\) increases, \(J(u_N)^{1/2}\) decays sharply, and the convergence speed is fast.

**4. Numerical Experiments**

In this section, we give numerical experiments to verify the efficiency of the least-squares non-polynomial finite element method.

**Example 2.** We set the period \(d\), the length of perfect conductive material strips \(s_1\), and the length of the slit \(s_2\) the same as in Example 1.

In figure 4 and figure 5, computations of our method are performed using MATLAB. In figure 4, with the wave number \(k = 1\), and the incident angle \(\theta = \pi / 3\). In each unit, take the number of bases \(N = 120\), the corresponding minimization functional \(J(u_N)^{1/2} = 2.2 \times 10^{-15}\). In figure 5, with
\( k = 20 \) and \( \theta = \pi / 6 \). In each unit, take \( N = 180 \), then \( J(u_0)^2 = 2.4 \times 10^{-13} \). We can see that with the increase of the wave number, the least-squares non-polynomial finite element method only needs to decompose a small computational domain and in every domain, we choose the appropriate bases to obtain the fast convergence.

Next, we show the results of our method and COMSOL FEM for comparison. In figure 6 and figure 7, the absolute values of the total field are shown with the wave number \( k = 100 \), and the incident angle \( \theta = 0 \). One can see that the results are almost the same. While in figure 6, our method costs 9.61 seconds with 1202 unknowns, and in figure 7, the COMSOL FEM costs 67 seconds with 213033 unknowns. We can see that with the number of unknowns and the calculation time, the least-squares non-polynomial finite element method is better than the FEM.

In theoretical analysis, the previous article shows the case where the length of the slit and the perfect conductive material strips are equal. For the case which the lengths are not equal, only some appropriate adjustments are needed to the domain decompose and approximate space. The method in this paper is still applicable, as given by the following example.

**Example 3.** Let the periodic strip gratings with period \( d = 4 \), the length of perfect conductive material strip is 3 and the length of the slit is 1 (figure 8). When the wave number \( k = 20 \) and the incident angle \( \theta = 0 \), the absolute value of the total field is shown in Figure 9.
5. Conclusion

In this paper, a least-squares non-polynomial finite element method is proposed for diffraction problem of strip gratings. It can be seen from the above experiments that as long as an appropriate number of bases is selected, the method need few elements, the operation speed is faster, less error in numerical results. And due to the large wave number, the algorithm is also efficient and highly accurate.

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References

[1] Bao, G. Cowsar, L. Masters, W. (2011) Mathematical Modeling in Optical Science. Tsinghua University Press, Beijing.
[2] Yin, W. Zhang, D. Ma, F. (2009) Numerical Calculation of the Scattering Problem for Grating by Integral Equation Method. Journal of Jilin University. Science Edition, 47(6): 1112-1120.
[3] Zhou, W. Wu, H. (2018) An Adaptive Finite Element Method for the Diffraction Grating Problem with PML and Few-Mode DtN Truncations. Journal of Scientific Computing, 76(3):1813-1838.
[4] Qin, W. Fang, D. (2001) Finite element method of solving diffraction problem of dielectric optical grating. Chinese journal of radio science, 16(4): 479-483.
[5] Feng, L. (2004) Wavelet-spectral methods for solving a class of Helmholtz equations with periodic coefficients. Journal of Natural Science of Heilongjiang University, 21(3):30-34.
[6] Babuska, I.M. Sauter, S.A. (2000) Is the pollution effect of the FEM avoidable for the Helmholtz equation considering high wave numbers?. Siam Review, 42: 451-484.
[7] Zheng, E. Ma, F. Zhang, D. (2013) A least-squares non-polynomial finite element method for solving the polygonal-line grating problem. J. Math. Anal. Appl, (397): 550-560.
[8] Zheng, E. Wang, Y. (2019) Galerkin method for the scattering problem of strip gratings. Advances in Difference Equations, 60.