

求解二维拟周期散射问题的两个谱方法

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摘要: 本文研究光学中的二维拟周期散射问题, 该问题由Helmholtz方程外加虚拟边界条件刻画。一个谱配置法和一个张量积谱方法被用来高精度自适应求解此问题。本文所提的方法可推广到求解一般的二维偏微分方程, 其中一个空间变量是周期的。数值例子显示这两个方法的有效性。

关键词: 谱方法, Helmholtz方程, 虚拟边界条件, Chebfun

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Two spectral methods for 2D quasi-periodic scattering problems

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Abstract: We consider the 2D quasi-periodic scattering problem in optics, which has been modelled by a boundary value problem governed by Helmholtz equation with transparent boundary conditions. A spectral collocation method and a tensor product spectral method are proposed to numerically solve the problem on rectangles. The discretization parameters can be adaptively chosen so that the numerical solution approximates the exact solution to a high accuracy. Our methods also apply to solve general partial differential equations in two space dimensions, one of which is periodic. Numerical examples are presented to illustrate the accuracy and efficiency of our methods.

Key words: Spectral method, Helmholtz equation, transparent boundary condition, Chebfun

0 Introduction

With the development of electromagnetic and optics technology and the increasing demands in industrial and military applications, scattering from periodic structures [1] have attracted much interest in recent years. A variety of numerical methods including finite difference methods [2], finite element methods [3, 4, 5, 6, 7, 8, 9, 10], spectral and spectral element methods [11, 12], integral equation methods [13, 14, 15, 16], Dirichlet-to-Neumann map methods

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[17], and mode expansion method [18, 19] have been developed by the engineering community and the applied mathematical community for solving linear diffraction problems from periodic structures.

Finite difference and finite element methods are easy to implement and result in sparse linear systems, which enable the use of sparse direct solvers. However, these methods typically have significant dispersion errors for high-frequency problems and thus fail to provide accurate solutions. If the medium is piecewise constant, boundary integral equations formulated on the interfaces of multilayer structures [16] or the boundaries of the obstacles [14, 15] are natural and mathematically rigorous. By exploiting high-order quadratures, one obtains much higher efficiency and accuracy than finite difference and finite element methods. For problems with general smooth media, spectral methods [20, 21, 22, 23, 24] can be employed. They are simple to implement and typically require relatively small number of unknowns to attain a fixed accuracy. We refer to [25] for a brief survey of existing spectral methods for partial differential equations.

In this paper, we consider 2D quasi-periodic scattering problems. By introducing transparent boundary conditions, the problem is governed by a Helmholtz equation with variable coefficients defined on rectangular domains. We propose a spectral collocation method and a tensor product spectral method. The first one uses the spectral collocation techniques [20, 21] and the second one, based on separable representations of the differential operator, combines the Fourier spectral method and the ultraspherical spectral method [26]. For vertically layered medium case, both methods only require to solve a one dimensional problem. The two spectral methods proposed in this paper can adaptively determine the number of unknowns and approximate the solution to a high accuracy. We remark that the tensor product spectral method leads to matrices that are banded or almost banded. By employing the fast algorithm in [26], a layered medium approximation problem can be used as a preconditioner for the problem with general media.

Recently, Chebfun software [27] was extended to solve problems in two dimensions [28, 25], both of which are nonperiodic. We refer to [29] for the summary of the mathematics and algorithms of Chebyshev technology for nonperiodic functions. Extension to periodic functions in one dimension was proposed in [30]. Our spectral methods can be used to solve the problems in two space dimensions, one of which is periodic. Implementing our methods with the adaptive strategies of Chebfun software is easy.

The rest of this paper is organized as follows. In §2 the model problem is formulated and further reduced to a boundary value problem. In §3 we present the spectral collocation method for the problem. Section 4 is devoted to the tensor product spectral method. Numerical examples illustrating the accuracy and efficiency of the methods are reported in §5. We present brief concluding remarks in §6.

1 Problem setting

Assume that no currents are present and that the fields are source free. Then the electromagnetic fields in the whole space are governed by the following time-harmonic Maxwell equations (time dependence $e^{-i\omega t}$)

$$\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad (1)$$

$$\nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}, \quad (2)$$

where $i = \sqrt{-1}$ is the imaginary unit, ω is the angular frequency, μ is the permeability, ε is the permittivity, \mathbf{E} is the electric field and \mathbf{H} is the magnetic field.

In this paper, we consider a simple quasi-periodic scattering model: μ is constant everywhere; ε is periodic in x variable of period 2π , invariant in z variable, and constant away from the region $|y| < 1 - \delta$, i.e., there exist constants ε^+ and ε^- such that

$$\begin{aligned} \varepsilon(x, y, z) &= \varepsilon^+, \text{ for } y > 1 - \delta, \\ \varepsilon(x, y, z) &= \varepsilon^-, \text{ for } y < \delta - 1. \end{aligned}$$

In the TM polarization, the electric field \mathbf{E} takes the simpler form

$$\mathbf{E}(x, y, z) = \mathbf{E}(x, y) = (0, 0, u(x, y)).$$

The Maxwell equations (1)-(2) yield the Helmholtz equation:

$$\Delta u + \omega^2 \varepsilon \mu u = 0. \quad (3)$$

Consider the plane wave $u^i = e^{i\alpha_0 x - i\beta_0 y}$ is incident from the above, where $\alpha_0 = \omega\sqrt{\varepsilon^+ \mu} \sin \theta$, $\beta_0 = \omega\sqrt{\varepsilon^+ \mu} \cos \theta$, and $-\pi/2 < \theta < \pi/2$ is the angle of incidence with respect to the positive y -axis. The incident wave u^i leads to reflected wave u^r and transmitted wave u^t . For $y > 1$, we have $u = u^i + u^r$, and for $y < -1$, $u = u^t$. We are interested in quasi-periodic solution u with phase $e^{i\alpha_0 2\pi}$, i.e., $ue^{-i\alpha_0 x}$ is 2π -periodic in x variable. Therefore, the reflected and transmitted waves can be written as

$$\begin{aligned} u^r &= \sum_{j \in \mathbb{Z}} r_j e^{i\alpha_j x + i\beta_j y}, \quad y > 1, \\ u^t &= \sum_{j \in \mathbb{Z}} t_j e^{i\alpha_j x - i\gamma_j y}, \quad y < -1, \end{aligned}$$

where r_j and t_j are unknown complex scalar coefficients and

$$\begin{aligned} \alpha_j &= \alpha_0 + j, \\ \beta_j &= \sqrt{\omega^2 \varepsilon^+ \mu - \alpha_j^2}, \quad \text{Im}(\beta_j) \geq 0, \\ \gamma_j &= \sqrt{\omega^2 \varepsilon^- \mu - \alpha_j^2}, \quad \text{Im}(\gamma_j) \geq 0. \end{aligned}$$

Note that if $\omega\sqrt{\varepsilon^+\mu}$ is real, then the j 's satisfying $\beta_j > 0$ correspond propagating modes. Throughout, we assume that $\beta_j \neq 0$ and $\gamma_j \neq 0$ for all $j \in \mathbb{Z}$. This assumption excludes the “resonant” cases, where waves can propagate along the x -axis.

For a quasi-periodic function $f(x)$, define the linear operators S and T by [31, 32, 33]

$$(Sf)(x) = \sum_{j \in \mathbb{Z}} i\beta_j f_j e^{i\alpha_j x}, \quad (4)$$

$$(Tf)(x) = \sum_{j \in \mathbb{Z}} i\gamma_j f_j e^{i\alpha_j x}, \quad (5)$$

where

$$f(x) = \sum_{j \in \mathbb{Z}} f_j e^{i\alpha_j x},$$

$$f_j = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-i\alpha_j x} dx.$$

Let ν denote the unit outward normal. We obtain transparent boundary conditions:

$$\partial_\nu u - Su = -2i\beta_0 e^{i\alpha_0 x - i\beta_0}, \quad \text{on } (0, 2\pi) \times \{1\}, \quad (6)$$

$$\partial_\nu u - Tu = 0, \quad \text{on } (0, 2\pi) \times \{-1\}. \quad (7)$$

The quasi-periodic scattering problem is to solve the Helmholtz equation (3) in the rectangular domain $\Omega := (0, 2\pi) \times (-1, 1)$ subject to the transparent boundary conditions (6)-(7) and the quasi-periodic boundary condition

$$u(x + 2\pi, y) = e^{i\alpha_0 2\pi} u(x, y). \quad (8)$$

Define $v = ue^{-i\alpha_0 x}$. Then v satisfies

$$\begin{cases} \Delta_{\alpha_0} v + \omega^2 \varepsilon \mu v = 0, & \text{in } \Omega = (0, 2\pi) \times (-1, 1), \\ \partial_y v - e^{-i\alpha_0 x} S(e^{i\alpha_0 x} v) = -2i\beta_0 e^{-i\beta_0}, & \text{on } (0, 2\pi) \times \{1\}, \\ \partial_y v + e^{-i\alpha_0 x} T(e^{i\alpha_0 x} v) = 0, & \text{on } (0, 2\pi) \times \{-1\}, \\ v(x + 2\pi, y) = v(x, y), & \text{in } \mathbb{R}^2, \end{cases} \quad (9)$$

where the operator Δ_{α_0} is defined by $\Delta_{\alpha_0} = \partial_{xx} + 2i\alpha_0 \partial_x - |\alpha_0|^2 + \partial_{yy}$. The solution to (9) is unique at all but a discrete set of frequencies ω when the incident angle θ is fixed. Existence and uniqueness of the solution is strictly proved in Dobson [34] by a variational approach.

Since the operators S and T given in (4)-(5) are defined by infinite series, the computation has to be truncated in practice. For simplicity, we truncate S and T as follows:

$$(S^N f)(x) = \sum_{j=1-q}^{N-q} i\beta_j f_j e^{i\alpha_j x},$$

$$(T^N f)(x) = \sum_{j=1-q}^{N-q} i\gamma_j f_j T^N e^{i\alpha_j x},$$

where N is a sufficiently large integer and q is an integer satisfying that $1 \leq q \leq N$ and all propagating modes are contained in the middle of the truncated series. Next, we propose two spectral methods for the following problem

$$\begin{cases} \Delta_{\alpha_0} v + \omega^2 \varepsilon \mu v = 0, & \text{in } \Omega = (0, 2\pi) \times (-1, 1), \\ \partial_y v - e^{-i\alpha_0 x} S^N(e^{i\alpha_0 x} v) = -2i\beta_0 e^{-i\beta_0}, & \text{on } (0, 2\pi) \times \{1\}, \\ \partial_y v + e^{-i\alpha_0 x} T^N(e^{i\alpha_0 x} v) = 0, & \text{on } (0, 2\pi) \times \{-1\}, \\ v(x + 2\pi, y) = v(x, y), & \text{in } \mathbb{R}^2. \end{cases} \quad (10)$$

We refer to [9, Section 3.1] for the discussion on the existence and uniqueness of the solution of the problem (10). In this paper, we focus on the accurate and efficient spectral methods for the problem (10). Thus we always assume that the discrete problem has a unique solution.

2 A spectral collocation method

We approximate the problem (10) by Fourier discretization in x variable and Chebyshev discretization in y variable. Let $x_n = nh$ and $y_m = \cos(m\pi/M)$ with $h = 2\pi/N$, $n = 1, 2, \dots, N$, and $m = 0, 1, \dots, M$. Introduce the first-order Fourier differentiation matrix [35, 36, 21], $\mathbf{D}_x = [d_{ij}^x]_{i,j=1}^N$,

$$\begin{aligned} N \text{ odd,} \quad d_{ij}^x &= \begin{cases} 0, & i = j, \\ (-1)^{i-j} \frac{1}{2} \csc \frac{(i-j)h}{2}, & i \neq j, \end{cases} \\ N \text{ even,} \quad d_{ij}^x &= \begin{cases} 0, & i = j, \\ (-1)^{i-j} \frac{1}{2} \cot \frac{(i-j)h}{2}, & i \neq j, \end{cases} \end{aligned}$$

the second-order Fourier differentiation matrix [35, 36, 21], $\mathbf{D}_{xx} = [d_{ij}^{xx}]_{i,j=1}^N$,

$$\begin{aligned} N \text{ odd,} \quad d_{ij}^{xx} &= \begin{cases} -\frac{\pi^2}{3h^2} + \frac{1}{12}, & i = j, \\ (-1)^{i-j+1} \frac{1}{2} \csc \frac{(i-j)h}{2} \cot \frac{(i-j)h}{2}, & i \neq j, \end{cases} \\ N \text{ even,} \quad d_{ij}^{xx} &= \begin{cases} -\frac{\pi^2}{3h^2} - \frac{1}{6}, & i = j, \\ (-1)^{i-j+1} \frac{1}{2} \csc^2 \frac{(i-j)h}{2}, & i \neq j, \end{cases} \end{aligned}$$

and the $(M+1) \times (M+1)$ Chebyshev differentiation matrix [37, 36, 21], $\mathbf{D}_y = [d_{ij}^y]_{i,j=0}^M$,

$$\begin{aligned} d_{00}^y &= \frac{2M^2+1}{6}, \quad d_{MM}^y = -\frac{2M^2+1}{6}, \\ d_{ii}^y &= -\frac{y_i}{2(1-y_i^2)}, \quad i = 1, \dots, M-1, \\ d_{ij}^y &= \frac{c_i}{c_j} \frac{(-1)^{i+j}}{(y_i - y_j)}, \quad i \neq j, \quad i, j = 0, 1, \dots, M, \\ c_i &= \begin{cases} 2, & i = 0 \text{ or } M, \\ 1, & \text{otherwise.} \end{cases} \end{aligned}$$

The discretization of the Helmholtz equation in (10) takes the form

$$\mathbf{PVD}_{xx}^T + 2i\alpha_0 \mathbf{PVD}_x^T - |\alpha_0|^2 \mathbf{PV} + \mathbf{PD}_y^2 \mathbf{V} + \omega^2 \mu \mathbf{P}(\varepsilon \odot \mathbf{V}) = \mathbf{0}, \quad (11)$$

where \mathbf{P} is the $(M-1) \times (M+1)$ matrix obtained by deleting the first and last rows of the identity matrix \mathbf{I}_{M+1} , $\mathbf{V} = [v_{mn}]_{m=0, n=1}^{M, N}$, v_{mn} is the approximate solution at the point (x_n, y_m) , $\varepsilon = [\varepsilon_{mn}]_{m=0, n=1}^{M, N}$, $\varepsilon_{mn} = \varepsilon(x_n, y_m)$, and \odot denotes the componentwise product. The operators $e^{-i\alpha_0 x} S^N(e^{i\alpha_0 x} \cdot)$ and $e^{-i\alpha_0 x} T^N(e^{i\alpha_0 x} \cdot)$ can be approximated by $N \times N$ matrices:

$$\mathbf{S} = \mathbf{G}^* \mathbf{\Lambda}_\beta \mathbf{G} := \mathbf{G}^* \text{diag}\{i\beta_{1-q}, i\beta_{2-q}, \dots, i\beta_{N-q}\} \mathbf{G}, \quad (12)$$

$$\mathbf{T} = \mathbf{G}^* \mathbf{\Lambda}_\gamma \mathbf{G} := \mathbf{G}^* \text{diag}\{i\gamma_{1-q}, i\gamma_{2-q}, \dots, i\gamma_{N-q}\} \mathbf{G}, \quad (13)$$

where \mathbf{G} is the $N \times N$ matrix with (i, j) entry $e^{-i2(i-q)j\pi/N}/\sqrt{N}$, $i, j = 1, \dots, N$. The discrete forms of the transparent boundary conditions are given by

$$\mathbf{e}_0^T \mathbf{D}_y \mathbf{V} - \mathbf{e}_0^T \mathbf{V} \mathbf{S}^T = -2i\beta_0 e^{-i\beta_0} \mathbf{e}^T, \quad (14)$$

$$\mathbf{e}_M^T \mathbf{D}_y \mathbf{V} + \mathbf{e}_M^T \mathbf{V} \mathbf{T}^T = \mathbf{0}, \quad (15)$$

where

$$\mathbf{e}_0 = [1 \ 0 \ \dots \ 0]^T \in \mathbb{R}^{M+1},$$

$$\mathbf{e}_M = [0 \ \dots \ 0 \ 1]^T \in \mathbb{R}^{M+1},$$

$$\mathbf{e} = [1 \ 1 \ \dots \ 1]^T \in \mathbb{R}^N.$$

Let

$$\mathbf{H} = (\mathbf{D}_{xx} + 2i\alpha_0 \mathbf{D}_x - |\alpha_0|^2 \mathbf{I}_N) \otimes \mathbf{P} + \mathbf{I}_N \otimes (\mathbf{PD}_y^2) + \omega^2 \mu (\mathbf{I}_N \otimes \mathbf{P}) \text{diag}\{\text{vec}(\varepsilon)\}. \quad (16)$$

Combining (11), (14) and (15) yields the linear system

$$\mathbf{A} \mathbf{v} = \mathbf{g}, \quad (17)$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{I}_N \otimes (\mathbf{e}_0^T \mathbf{D}_y) - \mathbf{S} \otimes \mathbf{e}_0^T \\ \mathbf{H} \\ \mathbf{I}_N \otimes (\mathbf{e}_M^T \mathbf{D}_y) + \mathbf{T} \otimes \mathbf{e}_M^T \end{bmatrix},$$

and

$$\mathbf{v} = \text{vec}(\mathbf{V}), \quad \mathbf{g} = \begin{bmatrix} -2i\beta_0 e^{-i\beta_0} \mathbf{e} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \in \mathbb{C}^{MN+N}.$$

Remark 1. The matrix \mathbf{P} in (11) is called the downsampling matrix [38] obtained by using the inner Chebyshev points of the second kind,

$$y_m = \cos\left(\frac{m\pi}{M}\right), \quad m = 1, 2, \dots, M-1,$$

as resampling points. One might choose other points, such as the Chebyshev points of the first kind,

$$y_m = \cos\left(\frac{(2m-1)\pi}{2(M-1)}\right), \quad m = 1, 2, \dots, M-1.$$

We refer to [39] for explicit construction of rectangular differentiation matrix \mathbf{PD}_y^2 .

2.1 Layered medium case

Assume that the medium in Ω is vertically layered, i.e., $\varepsilon(x, y) = \varepsilon(y)$. Then, the matrix \mathbf{H} in (16) takes the form

$$\mathbf{H} = (\mathbf{D}_{xx} + 2i\alpha_0 \mathbf{D}_x - |\alpha_0|^2 \mathbf{I}_N) \otimes \mathbf{P} + \mathbf{I}_N \otimes (\mathbf{P}(\mathbf{D}_y^2 + \omega^2 \mu \boldsymbol{\varepsilon}^y)),$$

where

$$\boldsymbol{\varepsilon}^y = \text{diag}\{\varepsilon(y_0), \varepsilon(y_1), \dots, \varepsilon(y_M)\}.$$

Let \mathbf{F} be the discrete Fourier transform matrix with (i, j) entry $e^{-i2(i-1)(j-1)\pi/N}/\sqrt{N}$, $i, j = 1, 2, \dots, N$. We have the following lemmas. The proofs are straightforward.

Lemma 1. The matrices \mathbf{S} in (12) and \mathbf{T} in (13) satisfy

$$\mathbf{S} = \mathbf{F}^* \boldsymbol{\Lambda}_S \mathbf{F}, \quad \mathbf{T} = \mathbf{F}^* \boldsymbol{\Lambda}_T \mathbf{F},$$

where

$$\begin{aligned} \boldsymbol{\Lambda}_S &= \text{diag}\{\lambda_1^\beta, \lambda_2^\beta, \dots, \lambda_N^\beta\} \\ &= \text{diag}\{i\beta_0, i\beta_1, \dots, i\beta_{N-q}, i\beta_{1-q}, i\beta_{2-q}, \dots, i\beta_{-1}\}, \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{\Lambda}_T &= \text{diag}\{\lambda_1^\gamma, \lambda_2^\gamma, \dots, \lambda_N^\gamma\} \\ &= \text{diag}\{i\gamma_0, i\gamma_1, \dots, i\gamma_{N-q}, i\gamma_{1-q}, i\gamma_{2-q}, \dots, i\gamma_{-1}\}. \end{aligned}$$

Lemma 2. *The first-order spectral differentiation matrix \mathbf{D}_x and the second-order spectral differentiation matrix \mathbf{D}_{xx} can be diagonalized by \mathbf{F} . Specifically, we have*

$$\mathbf{D}_x = \mathbf{F}^* \mathbf{\Lambda}_x \mathbf{F}, \quad \mathbf{D}_{xx} = \mathbf{F}^* \mathbf{\Lambda}_{xx} \mathbf{F},$$

where

$$\begin{aligned} \mathbf{\Lambda}_x &= \text{diag}\{\lambda_1^x, \lambda_2^x, \dots, \lambda_N^x\} \\ &= \begin{cases} i \cdot \text{diag}\{0, 1, \dots, (N-1)/2, (1-N)/2, (3-N)/2, \dots, -1\}, & \text{if } N \text{ is odd,} \\ i \cdot \text{diag}\{0, 1, \dots, N/2-1, 0, 1-N/2, 2-N/2, \dots, -1\}, & \text{if } N \text{ is even,} \end{cases} \end{aligned}$$

and

$$\begin{aligned} \mathbf{\Lambda}_{xx} &= \text{diag}\{\lambda_1^{xx}, \lambda_2^{xx}, \dots, \lambda_N^{xx}\} \\ &= \begin{cases} -\text{diag}\{0, 1, 4, \dots, ((N-1)/2)^2, ((1-N)/2)^2, \dots, 4, 1\}, & \text{if } N \text{ is odd,} \\ -\text{diag}\{0, 1, 4, \dots, (N/2)^2, (N/2-1)^2, \dots, 4, 1\}, & \text{if } N \text{ is even.} \end{cases} \end{aligned}$$

Multiplying the linear system (17) by

$$\begin{bmatrix} \mathbf{F} & & \\ & \mathbf{F} \otimes \mathbf{I}_{M-1} & \\ & & \mathbf{F} \end{bmatrix}$$

from the left yields

$$\begin{bmatrix} \mathbf{I}_N \otimes (\mathbf{e}_0^T \mathbf{D}_y) - \mathbf{\Lambda}_S \otimes \mathbf{e}_0^T \\ (\mathbf{\Lambda}_{xx} + 2i\alpha_0 \mathbf{\Lambda}_x - |\alpha_0|^2 \mathbf{I}_N) \otimes \mathbf{P} + \mathbf{I}_N \otimes (\mathbf{P}(\mathbf{D}_y^2 + \omega^2 \mu \epsilon^y)) \\ \mathbf{I}_N \otimes (\mathbf{e}_M^T \mathbf{D}_y) + \mathbf{\Lambda}_T \otimes \mathbf{e}_M^T \end{bmatrix} \hat{\mathbf{v}} = \hat{\mathbf{g}}, \quad (18)$$

where

$$\hat{\mathbf{v}} = (\mathbf{F} \otimes \mathbf{I}_{M+1}) \mathbf{v}, \quad \hat{\mathbf{g}} = \begin{bmatrix} -2i\beta_0 e^{-i\beta_0} \hat{\mathbf{e}} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \hat{\mathbf{e}} = \mathbf{F} \mathbf{e} = \begin{bmatrix} \sqrt{N} \\ \mathbf{0} \end{bmatrix}.$$

Reordering the unknowns and equations in (18), we obtain N uncoupled linear systems of order $M+1$:

$$\begin{bmatrix} \mathbf{e}_0^T \mathbf{D}_y - i\beta_0 \mathbf{e}_0^T \\ \mathbf{P}(\mathbf{D}_y^2 + \omega^2 \mu \epsilon^y) - |\alpha_0|^2 \mathbf{P} \\ \mathbf{e}_M^T \mathbf{D}_y + i\gamma_0 \mathbf{e}_M^T \end{bmatrix} \hat{\mathbf{v}}_1 = \begin{bmatrix} -2i\beta_0 e^{-i\beta_0} \sqrt{N} \\ \mathbf{0} \\ 0 \end{bmatrix}, \quad (19)$$

and for $i = 2, \dots, N$,

$$\begin{bmatrix} \mathbf{e}_0^T \mathbf{D}_y - \lambda_i^\beta \mathbf{e}_0^T \\ (\lambda_i^{xx} + 2i\alpha_0 \lambda_i^x - |\alpha_0|^2) \mathbf{P} + \mathbf{P}(\mathbf{D}_y^2 + \omega^2 \mu \epsilon^y) \\ \mathbf{e}_M^T \mathbf{D}_y + \lambda_i^\gamma \mathbf{e}_M^T \end{bmatrix} \hat{\mathbf{v}}_i = \mathbf{0},$$

where $\hat{\mathbf{v}}_i$ is the i th column of $\mathbf{V} \mathbf{F}^T$. Obviously, $\hat{\mathbf{v}}_i = \mathbf{0}$ for $i \neq 1$. After solving the linear system (19), we obtain \mathbf{v} by $\mathbf{v} = (\mathbf{F}^* \otimes \mathbf{I}_{M+1}) \hat{\mathbf{v}}$.

3 A tensor product spectral method

We propose a tensor product spectral method (see §4.3) for the problem (10) by combining the Fourier spectral method and the ultraspherical spectral method [26].

3.1 Fourier spectral method for periodic second-order linear ordinary differential equations

We consider the second-order linear ordinary differential equation (ODE)

$$\mathcal{L}w := a(x)w''(x) + b(x)w'(x) + c(x)w(x) = f(x), \quad x \in [0, 2\pi] \quad (20)$$

with periodic boundary conditions. Here, $a(x)$, $b(x)$, $c(x)$ and $f(x)$ are periodic functions on $[0, 2\pi]$. The Fourier spectral method finds an infinite vector

$$\mathbf{w} = \left[\cdots \quad w_{-2} \quad w_{-1} \quad w_0 \quad w_1 \quad w_2 \quad \cdots \right]^T,$$

such that the Fourier expansion of the solution of (20) is given by

$$w(x) = \sum_{j \in \mathbb{Z}} w_j e^{ijx}, \quad x \in [0, 2\pi].$$

Note that we have

$$w'(x) = \sum_{j \in \mathbb{Z}} ij w_j e^{ijx}, \quad w''(x) = \sum_{j \in \mathbb{Z}} (-j^2) w_j e^{ijx}.$$

The first-order differentiation operator is given by

$$\mathcal{D}_x = i \begin{bmatrix} \ddots & & & & & & \\ & -3 & & & & & \\ & & -2 & & & & \\ & & & -1 & & & \\ & & & & 0 & & \\ & & & & & 1 & \\ & & & & & & 2 \\ & & & & & & & 3 \\ & & & & & & & & \ddots \end{bmatrix},$$

and the second-order differentiation operator is given by \mathcal{D}_x^2 . In order to handle variable coefficients of the forms $a(x)w''(x)$, $b(x)w'(x)$ and $c(x)w(x)$ in (20), we need to represent the multiplication of two Fourier series as an operator on coefficients. Let $\mathcal{T}[a]$ denote the multiplication operator that represents multiplication of two Fourier series, i.e., if \mathbf{w} is a vector of

Fourier expansion coefficients of $w(x)$, then $\mathcal{T}[a]\mathbf{w}$ returns the Fourier expansion coefficients of $a(x)w(x)$. Suppose that $a(x)$ is given by its Fourier series

$$a(x) = \sum_{j \in \mathbb{Z}} a_j e^{ijx}.$$

Then the explicit formula for $\mathcal{T}[a]$ is given by the following Toeplitz operator

$$\mathcal{T}[a] = \begin{bmatrix} \ddots & \vdots & \ddots \\ \ddots & a_{-2} & \ddots \\ \ddots & a_{-1} & \ddots \\ \ddots & a_0 & \ddots \\ \ddots & a_1 & \ddots \\ \ddots & a_2 & \ddots \\ \ddots & \vdots & \ddots \end{bmatrix}.$$

This multiplication operator looks dense; however, if $a(x)$ is approximated by a *trigonometric polynomial of degree n* , then $\mathcal{T}[a]$ is banded with a bandwidth of n . Combining the differentiation and multiplication operators yields

$$(\mathcal{T}[a]\mathcal{D}_x^2 + \mathcal{T}[b]\mathcal{D}_x + \mathcal{T}[c])\mathbf{w} = \mathbf{f},$$

where \mathbf{w} and \mathbf{f} are vectors of Fourier expansion coefficients of $w(x)$ and $f(x)$, respectively. We need truncate the operator to derive a practical numerical scheme. Let \mathcal{P}_N be the projection operator satisfying

$$\mathcal{P}_N \mathbf{w} = \begin{bmatrix} \mathbf{0} & \mathbf{I}_N & \mathbf{0} \end{bmatrix} \mathbf{w} = \begin{bmatrix} w_{1-q} & w_{2-q} & \cdots & w_{N-q} \end{bmatrix}^T.$$

We obtain the following linear system

$$(\mathcal{P}_N \mathcal{L}^{\mathbb{D}} \mathcal{P}_N^T)(\mathcal{P}_N \mathbf{w}) = \mathcal{P}_N \mathbf{f},$$

where

$$\mathcal{L}^{\mathbb{D}} = \mathcal{T}[a]\mathcal{D}_x^2 + \mathcal{T}[b]\mathcal{D}_x + \mathcal{T}[c].$$

The truncation parameter N can be adaptively chosen so that the numerical solution approximates the exact solution to relative machine precision.

3.2 The ultraspherical spectral method [26] for second-order linear ordinary differential equations

Consider the second order linear ordinary differential equation

$$\mathcal{L}w := a(x)w''(x) + b(x)w'(x) + c(x)w(x) = f(x), \quad (21)$$

where $a(x)$, $b(x)$, $c(x)$, $w(x)$ and $f(x)$ are functions defined on $[-1, 1]$. The ultraspherical spectral method finds an infinite vector

$$\mathbf{w} = \begin{bmatrix} w_0 & w_1 & \cdots \end{bmatrix}^T$$

such that the Chebyshev expansion of the solution of (21) is given by

$$w(x) = \sum_{j=0}^{\infty} w_j T_j(x), \quad x \in [-1, 1],$$

where $T_j(x)$ is the degree j Chebyshev polynomial.

Note that we have the following recurrence relation

$$\frac{d^\lambda T_n}{dx^\lambda} = \begin{cases} 2^{\lambda-1} n(\lambda-1)! C_{n-\lambda}^{(\lambda)}, & n \geq \lambda, \\ 0, & 0 \leq n \leq \lambda-1, \end{cases}$$

where $C_j^{(\lambda)}$ is the ultraspherical polynomial with an integer parameter $\lambda \geq 1$ of degree j [40]. Then the differentiation operator for the λ th derivative is given by

$$\mathcal{D}_\lambda = 2^{\lambda-1}(\lambda-1)! \begin{bmatrix} \mathbf{0} & \lambda & & & \\ & \lambda+1 & & & \\ & & \lambda+2 & & \\ & & & \ddots & \\ & & & & \ddots \end{bmatrix}, \quad \lambda \geq 1. \quad (22)$$

Here $\mathbf{0}$ in (22) denotes a λ -dimensional zero row vector. The conversion operator converting a vector of Chebyshev expansion coefficients to a vector of $C^{(1)}$ expansion coefficients, denoted by \mathcal{S}_0 , and the conversion operator converting a vector of $C^{(\lambda)}$ expansion coefficients to a vector of $C^{(\lambda+1)}$ expansion coefficients, denoted by \mathcal{S}_λ , are given by

$$\mathcal{S}_0 = \begin{bmatrix} 1 & 0 & -\frac{1}{2} & & \\ & \frac{1}{2} & 0 & -\frac{1}{2} & \\ & & \frac{1}{2} & 0 & \ddots \\ & & & \frac{1}{2} & \ddots \\ & & & & \ddots \end{bmatrix}, \quad \mathcal{S}_\lambda = \begin{bmatrix} 1 & 0 & -\frac{\lambda}{\lambda+2} & & \\ & \frac{\lambda}{\lambda+1} & 0 & -\frac{\lambda}{\lambda+3} & \\ & & \frac{\lambda}{\lambda+2} & 0 & \ddots \\ & & & \frac{\lambda}{\lambda+3} & \ddots \\ & & & & \ddots \end{bmatrix}, \quad \lambda \geq 1.$$

We also require the multiplication operator $\mathcal{M}_0[a]$ that represents multiplication of two Chebyshev series, and the multiplication operator $\mathcal{M}_\lambda[a]$ that represents multiplication of two $C^{(\lambda)}$ series, i.e., if \mathbf{w} is a vector of Chebyshev expansion coefficients of $w(x)$, then $\mathcal{M}_0[a]\mathbf{w}$ returns the Chebyshev expansion coefficients of $a(x)w(x)$, and $\mathcal{M}_\lambda[a]\mathcal{S}_{\lambda-1} \cdots \mathcal{S}_0\mathbf{w}$ returns the $C^{(\lambda)}$ expansion coefficients of $a(x)w(x)$. Suppose that $a(x)$ has the Chebyshev expansion

$$a(x) = \sum_{j=0}^{\infty} a_j T_j(x).$$

Then $\mathcal{M}_0[a]$ can be written as [26]:

$$\mathcal{M}_0[a] = \frac{1}{2} \begin{bmatrix} 2a_0 & a_1 & a_2 & a_3 & \cdots \\ a_1 & 2a_0 & a_1 & a_2 & \ddots \\ a_2 & a_1 & 2a_0 & a_1 & \ddots \\ a_3 & a_2 & a_1 & 2a_0 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} + \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ a_1 & a_2 & a_3 & a_4 & \cdots \\ a_2 & a_3 & a_4 & a_5 & \ddots \\ a_3 & a_4 & a_5 & a_6 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

The explicit formula for the entries of $\mathcal{M}_\lambda[a]$ with $\lambda \geq 1$ is given in [26]. This multiplication operators $\mathcal{M}_\lambda[a]$ with $\lambda \geq 0$ look dense; however, if $a(x)$ is approximated by a truncation of its Chebyshev or $C^{(\lambda)}$ series, then $\mathcal{M}_\lambda[a]$ is banded. Combining the differentiation, conversion and multiplication operators yields

$$(\mathcal{M}_2[a]\mathcal{D}_2 + \mathcal{S}_1\mathcal{M}_1[b]\mathcal{D}_1 + \mathcal{S}_1\mathcal{S}_0\mathcal{M}_0[c])\mathbf{w} = \mathcal{S}_1\mathcal{S}_0\mathbf{f}, \quad (23)$$

where \mathbf{w} and \mathbf{f} are vectors of Chebyshev expansion coefficients of $w(x)$ and $f(x)$, respectively. We need truncate the operator to derive a practical numerical scheme. Let \mathcal{Q}_M be the projection operator given by

$$\mathcal{Q}_M = \begin{bmatrix} \mathbf{I}_M & \mathbf{0} \end{bmatrix}.$$

We obtain the following linear system

$$(\mathcal{Q}_M\mathcal{L}^{\mathbb{D}}\mathcal{Q}_M^T)(\mathcal{Q}_M\mathbf{w}) = (\mathcal{Q}_M\mathcal{S}_1\mathcal{S}_0\mathcal{Q}_M^T)(\mathcal{Q}_M\mathbf{f}),$$

where

$$\mathcal{L}^{\mathbb{D}} = \mathcal{M}_2[a]\mathcal{D}_2 + \mathcal{S}_1\mathcal{M}_1[b]\mathcal{D}_1 + \mathcal{S}_1\mathcal{S}_0\mathcal{M}_0[c].$$

3.3 Discretization of (10) for the special case $\varepsilon(x, y) = \phi(x)\psi(y)$

We seek the approximate solution $\tilde{v}(x, y)$ to the problem (10),

$$\tilde{v}(x, y) = \sum_{i=0}^{M-1} \sum_{j=1-q}^{N-q} v_{ij} e^{ijx} T_i(y).$$

The linear differential operator in (10) can be expressed as

$$\mathcal{L}^x \otimes \mathcal{I} + \mathcal{I} \otimes \mathcal{L}^y + \omega^2 \mu \phi \otimes \psi,$$

where $\mathcal{L}^x := \partial_{xx} + 2i\alpha_0\partial_x - |\alpha_0|^2$, $\mathcal{L}^y := \partial_{yy}$, \mathcal{I} is the identity operator, and ϕ and ψ are the corresponding multiplication operations. The discretization of the Helmholtz equation in (10) takes the form

$$\mathbf{QCVX}^T + \mathbf{QYV} + \omega^2 \mu \mathbf{Q}\Psi\mathbf{V}\Phi^T = \mathbf{0}, \quad (24)$$

where \mathbf{Q} is the $(M-2) \times M$ matrix obtained by deleting the last two rows of the identity matrix \mathbf{I}_M , $\mathbf{C} = \mathcal{Q}_M \mathcal{S}_1 \mathcal{S}_0 \mathcal{Q}_M^T$, $\mathbf{X} = \mathcal{P}_N (\mathcal{D}_x^2 + 2i\alpha_0 \mathcal{D}_x) \mathcal{P}_N^T - |\alpha_0|^2 \mathbf{I}_N$, $\mathbf{Y} = \mathcal{Q}_M \mathcal{D}_2 \mathcal{Q}_M^T$, $\mathbf{\Phi} = \mathcal{P}_N \mathcal{T}[\phi] \mathcal{P}_N^T$, $\mathbf{\Psi} = \mathcal{Q}_M \mathcal{S}_1 \mathcal{S}_0 \mathcal{M}_0[\psi] \mathcal{Q}_M^T$, $\mathbf{V} = [v_{ij}]_{i=0, j=1-q}^{M-1, N-q}$. The discrete forms of the transparent boundary conditions are given by

$$\mathbf{b}_1^T \mathbf{V} - \mathbf{a}_1^T \mathbf{V} \mathbf{\Lambda}_\beta = -2i\beta_0 e^{-i\beta_0} \mathbf{e}_q^T, \quad (25)$$

$$\mathbf{b}_2^T \mathbf{V} + \mathbf{a}_2^T \mathbf{V} \mathbf{\Lambda}_\gamma = \mathbf{0}, \quad (26)$$

where

$$\begin{aligned} \mathbf{\Lambda}_\beta &= \text{diag}\{i\beta_{1-q}, i\beta_{2-q}, \dots, i\beta_{N-q}\}, \\ \mathbf{\Lambda}_\gamma &= \text{diag}\{i\gamma_{1-q}, i\gamma_{2-q}, \dots, i\gamma_{N-q}\}, \\ \mathbf{b}_1 &= [0 \ 1 \ 4 \ \dots \ (M-1)^2]^T, \\ \mathbf{b}_2 &= [0 \ 1 \ -4 \ \dots \ (-1)^M (M-1)^2]^T, \\ \mathbf{a}_1 &= [1 \ 1 \ \dots \ 1]^T \in \mathbb{R}^M, \\ \mathbf{a}_2 &= [1 \ -1 \ \dots \ (-1)^{(M-1)}]^T \in \mathbb{R}^M, \end{aligned}$$

and \mathbf{e}_q is the q th column of the identity matrix \mathbf{I}_N .

Let

$$\mathbf{H} = \mathbf{X} \otimes (\mathbf{Q}\mathbf{C}) + \mathbf{I}_N \otimes (\mathbf{Q}\mathbf{Y}) + \omega^2 \mu \mathbf{\Phi} \otimes (\mathbf{Q}\mathbf{\Psi}). \quad (27)$$

Combining (24), (25) and (26) yields the linear system

$$\mathbf{A}\mathbf{v} = \mathbf{g}, \quad (28)$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{I}_N \otimes \mathbf{b}_1^T - \mathbf{\Lambda}_\beta \otimes \mathbf{a}_1^T \\ \mathbf{I}_N \otimes \mathbf{b}_2^T + \mathbf{\Lambda}_\gamma \otimes \mathbf{a}_2^T \\ \mathbf{H} \end{bmatrix},$$

and

$$\mathbf{v} = \text{vec}(\mathbf{V}), \quad \mathbf{g} = \begin{bmatrix} -2i\beta_0 e^{-i\beta_0} \mathbf{e}_q \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \in \mathbb{C}^{MN}.$$

Remark 2. For general bivariate function $\varepsilon(x, y)$, we can use its low rank approximant, i.e., sum of functions of the form $\phi(x)\psi(y)$, where $\phi(x)$ and $\psi(y)$ are univariate functions. An algorithm [28, 41] which is mathematically equivalent to Gaussian elimination with complete pivoting can be used to construct low rank approximations.

3.3.1 Layered medium case

In this case, we have $\varepsilon(x, y) = \psi(y)$, i.e., $\phi(x) = 1$. Then $\Phi = \mathbf{I}_N$. The matrix \mathbf{H} in (27) takes the form

$$\mathbf{H} = \mathbf{X} \otimes (\mathbf{Q}\mathbf{C}) + \mathbf{I}_N \otimes (\mathbf{Q}\mathbf{Y} + \omega^2 \mu \mathbf{Q}\Psi).$$

Reordering the unknowns and equations in (28), we obtain

$$\begin{bmatrix} \mathbf{b}_1^T - i\beta_0 \mathbf{a}_1^T \\ \mathbf{b}_2^T + i\gamma_0 \mathbf{a}_2^T \\ \mathbf{Q}(\mathbf{Y} + \omega^2 \mu \Psi - |\alpha_0|^2 \mathbf{C}) \end{bmatrix} \mathbf{v}_q = \begin{bmatrix} -2i\beta_0 e^{-i\beta_0} \\ 0 \\ \mathbf{0} \end{bmatrix}, \quad (29)$$

and

$$\begin{bmatrix} \mathbf{b}_1^T - i\beta_{j-q} \mathbf{a}_1^T \\ \mathbf{b}_2^T + i\gamma_{j-q} \mathbf{a}_2^T \\ \mathbf{Q}(\mathbf{Y} + \omega^2 \mu \Psi - ((j-q)^2 + 2\alpha_0(j-q) + |\alpha_0|^2) \mathbf{C}) \end{bmatrix} \mathbf{v}_j = \mathbf{0}, \quad j \neq q, \quad (30)$$

where \mathbf{v}_j is the j th column of \mathbf{V} . Obviously, $\mathbf{v}_j = \mathbf{0}$ for $j \neq q$.

Note that the fast algorithm in [26] can be used to solve the linear system (29), which requires $\mathcal{O}(m^2 M)$ operations. Here, m is the number of Chebyshev points needed to resolve the function $\psi(y)$. The coefficient matrix resulting from a layered medium approximation problem can be used as a preconditioner for the problem with general medium. The corresponding computational complexity for the preconditioner solve is $\mathcal{O}(m^2 MN)$.

4 Numerical results

We have performed numerical experiments in numerous cases. In this section, we present a few typical results of these experiments to illustrate the accuracy and efficiency of the two spectral methods. All computations are performed with MATLAB R2012a.

Example 1: A constant coefficient problem

The parameters are chosen as $\theta = \pi/3$, $\varepsilon = 1$ and $\mu = 1$ everywhere. All the right hand sides are chosen such that the exact solution is

$$u(x, y) = e^{\sin x + i\omega x \sin \theta} \sin(\omega y \cos \theta).$$

This simple example is used to test the accuracy of our methods. In Figure 1 we plot the real part of the solution for $\omega = 10\pi$. In Figure 2 we present the error in the maximum norm defined by

$$\text{Max Error} = \max_{m,n} |u(x_n, y_m) - \tilde{u}_{mn}|,$$

where \tilde{u}_{mn} is the computed solution at the point (x_n, y_m) obtained by the spectral collocation method in §3, and the error in the L^2 norm defined by

$$\|u(x, y) - \tilde{u}(x, y)\|_{L^2(\Omega)} = \left(\int_0^{2\pi} \int_{-1}^1 |u(x, y) - \tilde{u}(x, y)|^2 dx dy \right)^{1/2},$$

where $\tilde{u}(x, y)$ is the computed solution obtained by the tensor product spectral method in §4. The errors show that the solution is rapidly resolved once π degrees of freedom per wavelength are used (in agreement with the results from [25]). As a comparison, by the finite difference method proposed in [2] for a 512×256 uniform mesh, the error for the case $\omega = 10\pi$ is 5.51×10^{-2} .

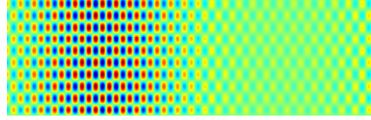


图 1: Real part of the exact solution of Example 1 with $\omega = 10\pi$.

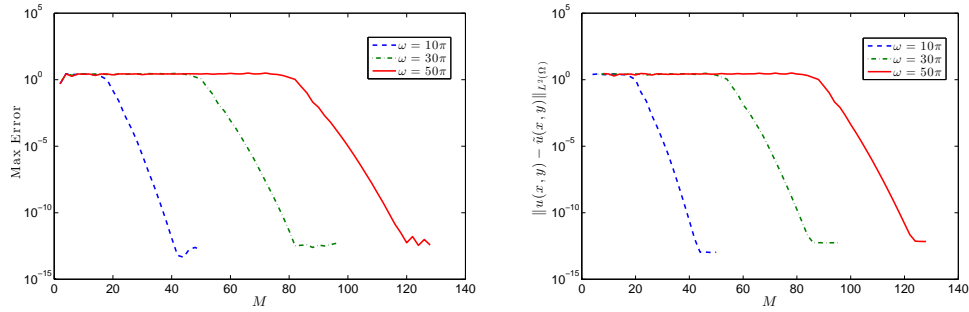


图 2: Errors in the maximum norm by the spectral collocation method (left) and the L^2 norm by the tensor product spectral method (right) for $\omega = 10\pi, 30\pi, 50\pi$.

Example 2: Variable coefficient problems

The parameters are chosen as $\theta = 3\pi/7$, $\omega = 10$, $\varepsilon^+ = \varepsilon^- = 1$, $\mu = 1$. We consider three cases:

$$\begin{aligned} \varepsilon_1(x, y) &= \varepsilon(y) = 1 + e^{\frac{3}{y^2-1}+4}, \\ \varepsilon_2(x, y) &= 1 + e^{\frac{3}{y^2-1}+4-\cos(\pi \sin(x/2))}, \\ \varepsilon_3(x, y) &= 1 + e^{\frac{3}{y^2-1}+4-y \cos(\pi \sin(x/2))}. \end{aligned}$$

The medium characterized by $\varepsilon_1(x, y)$ is vertically layered. Numerical methods for layered medium case are used to solve the corresponding problems. The bivariate medium function $\varepsilon_2(x, y)$ is of rank 2. We use the rank 7 approximant obtained by the algorithm proposed in [28, 41] to approximate the medium function $\varepsilon_3(x, y)$. In Figure 3, we plot the three media and the real parts of the corresponding waves obtained by our spectral methods. We observe that the numerical results obtained by the two methods coincide well for all the three media, which illustrates that the tensor product spectral method also works well when the medium is approximated by its low-rank approximant.

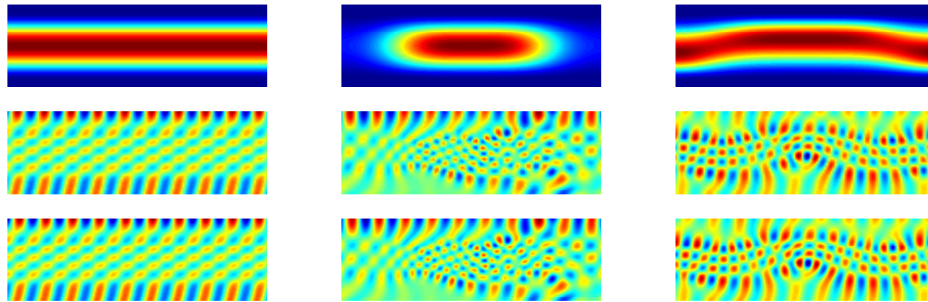


图 3: Media (Top) and corresponding real parts of the waves obtained by the spectral collocation method (Middle) and by the tensor product spectral method (Bottom). From left to right: numerical results for $\varepsilon_1(x, y)$, $\varepsilon_2(x, y)$, and $\varepsilon_3(x, y)$, respectively.

We also test the performance of the problem with $\varepsilon_1(x, y)$ as a preconditioner for the problem with $\varepsilon_3(x, y)$. The fast algorithm in [26] is used to solve the linear systems (29) and (30). The GMRES algorithm [42] is used as the iterative solver. The initial guess is set to be the zero vector. GMRES with the layered medium preconditioner obtained a solution with the relative residual norm less than 10^{-8} at the 37th iteration, while GMRES without preconditioning almost stagnates; see Figure 4 for the convergence history.

5 Concluding remarks

We have proposed a spectral collocation method and a tensor product spectral method for solving the 2D quasi-periodic scattering problem. Both of the methods can adaptively determine the number of unknowns and approximate the solution to a high accuracy. The tensor product spectral method is more interesting because it leads to matrices that are banded or almost banded, which enable the use of the fast, stable direct solver [26]. Based on this fast solver, a layered medium preconditioning technique is used to solve the problem with general media. Our methods also apply to solve general partial differential equations in two space dimensions,

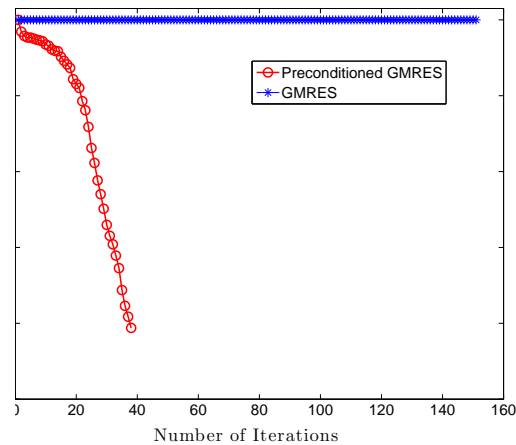


图 4: Convergence history for GMRES applied to the linear system (28).

one of which is periodic. Extension of our methods to bi-periodic structure diffraction grating problem [43] is being considered.

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