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Efficient Chebyshev Spectral Method for Solving Linear Elliptic PDEs Using Quasi-Inverse Technique

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Abstract. We present a systematic and efficient Chebyshev spectral method using quasi-inverse technique to directly solve the second order equation with the homogeneous Robin boundary conditions and the fourth order equation with the first and second boundary conditions. The key to the efficiency of the method is to multiply quasi-inverse matrix on both sides of discrete systems, which leads to band structure systems. We can obtain high order accuracy with less computational cost. For multi-dimensional and more complicated linear elliptic PDEs, the advantage of this methodology is obvious. Numerical results indicate that the spectral accuracy is achieved and the proposed method is very efficient for 2-D high order problems.

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1. Introduction

Due to high order accuracy, spectral methods have gained increasing popularity for several decades, especially in the field of computational fluid dynamics (see, e.g., [1, 2] and the references therein). According to different test functions in a variational formulation, there are three most common spectral schemes, namely, the collocation, Galerkin and tau methods. Since the collocation methods approximate differential equations in physical space, it is very easy to implement and adaptable to various of problems, including variable coefficient and nonlinear differential equations. Weideman and Reddy constructed a MATLAB software suit to solve differential equations by the spectral collocation methods in [13]. Trefethen's book [12] explained the essentials of spectral collocation methods with the aid of 40 short MATLAB programs. For multi-dimensional problems, the spectral collocation methods discretize the differential operators employing Kronecker products. In

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the Galerkin method, we work in the spectral space, it may lead to well conditioned linear systems with sparse matrices for problems with constant coefficients by choosing proper basis functions (see, e.g., [3,5,9,10]).

Although the collocation and Galerkin methods usually lead to optimal error estimates, the primary drawback of collocation method is that the differentiation matrices are dense in all dimensions, and it is generally not feasible to solve multi-dimensional problems by employing the Galerkin method. Shen used a matrix diagonalization method to solve the 2-D and 3-D Helmholtz problems in [9] and [10], but an eigenvalue-eigenvector decomposition of the discretized linear operator is required. Therefore it can only be used for relatively simple differential equations. Heinrichs [6] utilized a Galerkin basis set to obtain efficient differentiation matrices, and exploited the inherent structure of both the Galerkin differentiation matrices and the relationship between the Chebyshev and Galerkin spectral coefficients to maximize the sparsity of differential operators. Julien and Watson [7] presented the quasi-inverse technique to efficiently solve linear elliptic differential equations with constant coefficients under Dirichlet boundary conditions. In this paper, we present an extension of the Chebyshev spectral method using quasi-inverse technique to directly solve the Helmholtz equation with the homogeneous Robin boundary conditions and the general biharmonic equation with the first and second boundary conditions. For the general biharmonic equation, we give a uniform treatment for the first and second boundary conditions.

The main idea is that we employ a truncated series of Chebyshev polynomials to approximate the unknown function, and the differential operator is expanded by Chebyshev polynomials which vector of coefficients is represented by the product of derivative matrix and vector of Chebyshev coefficients of unknown function. The coefficients of this series are taken to be equal to the coefficients of the right-hand side expansion. According to Galerkin basis satisfying boundary conditions, we identify a transformation matrix which transforms the Chebyshev and Galerkin coefficients, and then multiply a quasi-inverse matrix on both sides of the resulting spectral system to obtain a pre-multiplied system $A\bar{v} = B\bar{f}$, where A and B have band structure. After we solve this system of equations, the Galerkin spectral coefficients are converted back to Chebyshev spectral coefficients. We obtain the approximation solution from spectral space to physical space using the forward Chebyshev transform by FFT.

The remainder of the paper is organized as follows. In the next section, we introduce some notations and summarize a few mathematical facts used in the remainder of the paper. In Section 3, we consider the Helmholtz equations for one, two and three dimensional cases. In Section 4, we study the general biharmonic equations for one and two dimensional cases. In Section 5, we present some numerical results. Finally, some concluding remarks are given in Section 6.

2. Preliminaries

2.1. Notation

We introduce some basic notations as follows:

- δ_{mn}, Kronecker-delta function, equal to 1 if $m = n$ and zero otherwise
- $\otimes$, Kronecker matrix product
- $T_m(x)$, mth degree Chebyshev polynomial
- $\bar{u}$, vector of spectral coefficients associated with Chebyshev spectral modes
- $\bar{v}$, vector of spectral coefficients associated with Galerkin spectral modes
- I_x, identity matrix with respect to x
- $I_x^{(\pm z)}$, quasi-identity matrix with respect to x. It is an identity matrix with z rows of zeros at the top/bottom for $\pm\, z$, respectively
- D_x^p, pth differential matrix with respect to x
- D_x^{-p}, pth quasi-inverse matrix for D_x^p
- $E_x^{(\pm z)}$, "shifted identity" matrix with ones on the $\pm z$ super/sub-diagonal for the variable x
- $S_x^{\{v\}}$, transformation matrix for the unknown v in the x spatial direction. It is used to transform between Chebyshev spectral coefficients and Galerkin spectral coefficients

2.2. Chebyshev polynomials

The Chebyshev polynomials can be represented by trigonometric functions

$$T_m(x) = \cos m\theta, \quad \theta = \arccos x,$$

which satisfy the orthogonality relation

$$(T_m(x), T_n(x))_\omega = \frac{c_m \pi}{2}\delta_{mn}, \tag{2.1}$$

where the weight function $\omega(x) = (1-x^2)^{-\frac{1}{2}}$, and $c_0 = 2$ and $c_m = 1$ for $m \geq 1$. The derivative of the Chebyshev polynomials can be represented by

$$T'_m(x) = \frac{m \sin(m\theta)}{\sin\theta}.$$

According to the trigonometric identity

$$2\sin\theta\cos m\theta = \sin(m+1)\theta - \sin(m-1)\theta,$$

we can obtain the following relation

$$2T_m(x) = \frac{T'_{m+1}(x)}{m+1} - \frac{T'_{m-1}(x)}{m-1}, \qquad m > 1. \tag{2.2}$$

The Chebyshev expansion of a function $u \in L^2_\omega(-1,1)$ is

$$u(x) = \sum_{m=0}^{\infty} \hat{u}_m T_m(x), \qquad \hat{u}_m = \frac{2}{\pi c_m}\int_{-1}^{1} u(x) T_m(x)\omega(x)dx. \tag{2.3}$$

The derivative of u expanded in Chebyshev polynomials can be represented formally as

$$u'(x) = \sum_{m=0}^{\infty} \hat{u}_m^{(1)} T_m(x), \tag{2.4}$$

where

$$\hat{u}_m^{(1)} = \frac{2}{c_m} \sum_{\substack{p=m+1 \\ p+m \ odd}}^{\infty} p\hat{u}_p, \qquad m \geq 0. \tag{2.5}$$

This expression is a consequence of the relation (2.2). From (2.2) one has

$$2m\hat{u}_m = c_{m-1}\hat{u}_{m-1}^{(1)} - \hat{u}_{m+1}^{(1)}, \qquad m \geq 1, \tag{2.6}$$

and from (2.6), we have the following recursion relation

$$c_m \hat{u}_m^{(1)} = 2(m+1)\hat{u}_{m+1} + \hat{u}_{m+2}^{(1)}, \qquad m \geq 0, \tag{2.7}$$

which yields (2.5). The generalization of this relation is [2]

$$c_m \hat{u}_m^{(q)} = 2(m+1)\hat{u}_{m+1}^{(q-1)} + \hat{u}_{m+2}^{(q)}, \qquad m \geq 0. \tag{2.8}$$

Similarly, the second derivative of u is expanded by Chebyshev polynomials

$$u''(x) = \sum_{m=0}^{\infty} \hat{u}_m^{(2)} T_m(x). \tag{2.9}$$

Due to the recursion relation (2.8), the coefficients are

$$\hat{u}_m^{(2)} = \frac{1}{c_m} \sum_{\substack{p=m+2 \\ p+m \ even}}^{\infty} p(p^2 - m^2)\hat{u}_p, \qquad m \geq 0. \tag{2.10}$$

Here, we can define a differential matrix D_x^2 such that $\bar{u}^{(2)} = D_x^2 * \bar{u}$, where D_x^2 is an upper triangular matrix with zeros on the main diagonal, $\bar{u}^{(2)}$ and $\bar{u}$ are the vectors of $\hat{u}_m^{(2)}$ and $\hat{u}_m$, respectively.

2.3. Quasi-inverse matrix

Definition 2.1. *D_x^{-p} is called the quasi-inverse matrix of order p associated with D_x^p in the x spatial direction, if $D_x^{-p} * D_x^p = I_x^{(p)}$ and $D_x^p * D_x^{-p} = I_x^{(-p)}$.*

The following properties of the quasi-inverse matrix can be found in [7].

Property 1. *A necessary condition of the definition of the quasi-inverse is that the matrix D_x^{-p} has zeros in the first p rows and the last p columns.*

Property 2. *Structure from the basis polynomials translates to the quasi-inverse representation such that there is a well defined structure between different order operators, (1)* $D_x^2 = D_x * D_x$, *(2)* $D_x^{-p} = I_x^{(p)} * D_x^{-p} * I_x^{(-p)}$, *(3)* $D_x^{-p} * D_x^q \equiv I_x^{(p)} * D_x^{-p+q}$.

The quasi-inverse matrix D^{-1} associated with D^1 is a tri-diagonal matrix whose nonzero entries defined by the three term recursion relation (2.6) are:

$$\left.\begin{array}{ll} \dot{d}_{m,m-1} = \dfrac{c_{m-1}}{2m}, & \text{sub-diagonal} \\ \dot{d}_{m,m+1} = -\dfrac{e_{m+2}}{2m}, & \text{super-diagonal} \end{array}\right\} \quad 1 \le m \le M. \tag{2.11}$$

The quasi-inverse matrix D^{-2} associated with D^2 is a penta-diagonal matrix whose nonzero elements are [4]:

$$\left.\begin{array}{ll} \dot{d}_{m,m-2} = \dfrac{c_{m-2}}{4m(m-1)}, & \text{2nd sub-diagonal} \\ \dot{d}_{m,m} = -\dfrac{e_{m+2}}{2(m^2-1)}, & \text{main diagonal} \\ \dot{d}_{m,m+2} = \dfrac{e_{m+4}}{4m(m+1)}, & \text{2nd super-diagonal} \end{array}\right\} \quad 2 \le m \le M, \tag{2.12}$$

where $e_m = 1$ for $m \le M$, $e_m = 0$ for $m > M$. The non-zero entries of D_x^{-p} are defined analytically by the three term recursion relation

$$c_m \hat{u}_m^{(q)} - \hat{u}_{m+2}^{(q)} = 2(m+1)\hat{u}_{m+1}^{(q-1)}, \qquad m \ge 0. \tag{2.13}$$

2.4. Kronecker products

Definition 2.2. *If* A *and* B *are of dimensions* $p \times q$ *and* $r \times s$*, respectively, then the Kronecker product* $A \otimes B$ *is the matrix of dimension* $pr \times qs$ *with* $p \times q$ *block form, where the* i,j *block is* $a_{ij}B$.

Property 3. *If* $A * C$ *and* $B * D$ *exist, then* $(A \otimes B) * (C \otimes D) = (A * C) \otimes (B * D)$.

In multiple dimensions, we can separate the differential operator by employing the Kronecker product. For instance, consider the discretization of the 2nd derivative operator in 1-D, 2-D and 3-D shown below:

- 1D $u_{xx}(x) \to D_x^2 * \bar{u}$
- 2D $u_{xx}(x,y) \to (D_x^2 \otimes I_y) * \bar{u}$
- 2D $u_{xy}(x,y) \to (D_x^1 \otimes D_y^1) * \bar{u}$
- 2D $u_{yy}(x,y) \to (I_x \otimes D_y^2) * \bar{u}$
- 3D $u_{xx}(x,y,z) \to (D_x^2 \otimes I_y \otimes I_z) * \bar{u}$
- 3D $u_{xy}(x,y,z) \to (D_x^1 \otimes D_y^1 \otimes I_z) * \bar{u}$, etc.

3. Helmholtz equations

In this section, we are interested in employing the Chebyshev spectral method using quasi-inverse technique to solve the Helmholtz equation

$$\alpha u - \triangle u = f, \quad \text{in } \Omega = I^d, \tag{3.1}$$

where $I = (-1,1)$ and $d = 1,2,3$.

3.1. 1-D Helmholtz

Let us begin with the one dimensional Helmholtz equation

$$\alpha u(x) - u''(x) = f(x), \qquad x \in I, \tag{3.2}$$

with the homogeneous Robin boundary condition

$$a_\pm u(\pm 1) + b_\pm u'(\pm 1) = 0. \tag{3.3}$$

We first expand $u(x)$, $u''(x)$ and $f(x)$ in terms of Chebyshev polynomials respectively

$$u_M(x) = \sum_{m=0}^{M} \hat{u}_m T_m(x), \qquad \bar{u} = (\hat{u}_0, \hat{u}_1, \cdots, \hat{u}_M)^T, \tag{3.4}$$

$$u''_M(x) = \sum_{m=0}^{M} \hat{u}_m^{(2)} T_m(x), \qquad \bar{u}^{(2)} = (\hat{u}_0^{(2)}, \hat{u}_1^{(2)}, \cdots, \hat{u}_M^{(2)})^T, \tag{3.5}$$

$$f_M(x) = \sum_{m=0}^{M} \hat{f}_m T_m(x), \qquad \bar{f} = (\hat{f}_0, \hat{f}_1, \cdots, \hat{f}_M)^T, \tag{3.6}$$

where

$$\hat{u}_m^{(2)} = \frac{1}{c_m} \sum_{\substack{p=m+2 \\ p+m \text{ even}}}^{M} p(p^2 - m^2)\hat{u}_p. \tag{3.7}$$

In spectral-Galerkin method, it is essential to seek an appropriate basis functions to satisfy the boundary condition. We usually choose a compact combination of Chebyshev polynomials as basis function. The following lemma provides a basis function which satisfies the homogeneous Robin boundary condition [11].

Lemma 3.1. *Let us define*

$$\begin{aligned} a_m =& -\{(a_+ + b_+(m+2)^2)(-a_- + b_- m^2) \\ & - (a_- - b_-(m+2)^2)(-a_+ - b_+ m^2)\}/DET_m, \\ b_m =& \{(a_+ + b_+(m+1)^2)(-a_- + b_- m^2) \\ & + (a_- - b_-(m+1)^2)(-a_+ - b_+ m^2)\}/DET_m, \end{aligned} \tag{3.8}$$

with

$$DET_m = 2a_+a_- + (m+1)^2(m+2)^2(a_-b_+ - a_+b_- - 2b_-b_+). \tag{3.9}$$

If $DET_m \neq 0$, then a linear combination of Chebyshev polynomials

$$\phi_m(x) = T_m(x) + a_m T_{m+1}(x) + b_m T_{m+2}(x) \tag{3.10}$$

satisfies the homogeneous Robin boundary condition (3.3).

Proof. Since $T_m(\pm1) = (\pm1)^m$ and $T'_m(\pm1) = (\pm1)^{m-1}m^2$, the boundary condition (3.3) leads to the following system for $\{a_m, b_m\}$:

$$\begin{aligned}
&(a_+ + b_+(m+1)^2)a_m + (a_+ + b_+(m+2)^2)b_m = -a_+ - b_+m^2,\\
&-(a_- - b_-(m+1)^2)a_m + (a_- - b_-(m+2)^2)b_m = -a_- + b_-m^2,
\end{aligned} \tag{3.11}$$

whose determinant DET_m is given by (3.9). When $DET_m \neq 0$, $\{a_m, b_m\}$ can be uniquely determined from (3.11). □

Remark 3.1. We note in particular that

- If $a_\pm = 1$ and $b_\pm = 0$ (Dirichlet boundary condition), we have $a_m = 0, b_m = -1$. Hence, $\phi_m(x) = T_m(x) - T_{m+2}(x)$ satisfies the homogeneous Dirichlet boundary condition.
- If $a_\pm = 0$ and $b_\pm = 1$ (Neumann boundary condition), we have

  $$a_m = 0, \qquad b_m = -\frac{m^2}{(m+2)^2}.$$

  Hence,

  $$\phi_m(x) = T_m(x) - \frac{m^2}{(m+2)^2}T_{m+2}(x)$$

  satisfies the homogeneous Neumann boundary condition.

We choose $\{\phi_m\}_{m=0}^{M-2}$ as Galerkin basis function and represent $u(x)$ in terms of a truncated series of Galerkin basis function:

$$u_M(x) = \sum_{m=0}^{M-2} \tilde{u}_m \phi_m(x), \quad \bar{v} = (\tilde{u}_0, \tilde{u}_1, \cdots, \tilde{u}_{M-2})^T. \tag{3.12}$$

Since the Galerkin basis function $\phi_m(x)$ are linear combinations of Chebyshev polynomials, the Chebyshev coefficients $\hat{u}_m$ are also linear combinations of the coefficients $\tilde{u}_m$, we try to seek a transformation matrix S_x, between the Chebyshev and Galerkin spectral representation such that

$$\bar{u} = S_x * \bar{v}. \tag{3.13}$$

Here $\bar{v}$ should be added two fictitious modes $\tilde{u}_{M-1}$ and $\tilde{u}_M$, which we specify to be identically zero, since S_x is $(M+1) \times (M+1)$.

To determine the appropriate transformation matrix S_{x_i}, we first project onto each $T_n(x)$ mode by applying inner products to each side defined by (2.1),

$$\begin{aligned}(\phi_m(x), T_n(x))_\omega =&(T_m(x) + a_m T_{m+1}(x) + b_m T_{m+2}(x), T_n(x))_\omega \\ =&\frac{c_m \pi}{2}\delta_{mn} + a_m \frac{c_{m+1}\pi}{2}\delta_{m+1,n} + b_m \frac{c_{m+2}\pi}{2}\delta_{m+2,n}.\end{aligned} \tag{3.14}$$

We can express this inner product relation in terms of shifted identity matrices $E_x^{(k)} \equiv [e_{m,n}] \equiv [\delta_{m,n-k}]$. For $k < 0$, $E_x^{(k)}$ defines a square matrix $(M+1) \times (M+1)$ with ones on the kth sub-diagonal, whereas for $k > 0$, the identity matrix $I_x = [\delta_{m,n}]$ is equivalent to $E_x^{(0)}$. A matrix with entries $[e_{m,n} \equiv \delta_{m,n+1}]$ can be represented by $E_x^{(-1)}$. We define the following transformation matrix for the Robin boundary condition,

$$S_x = E_x^{(0)} + E_x^{(-1)} W_1 + E_x^{(-2)} W_2, \tag{3.15}$$

where W_1 and W_2 are the weight matrices with diagonal entries $\{a_m\}$ and $\{b_m\}$, respectively.

The transformation matrix provides a convenient means for discretizing the differential equation with the boundary conditions embedded within the differentiation matrix. The discrete 1-D Helmholtz system of equations in spectral space is

$$(\alpha I_x - D_x^2) * S_x * \bar{v} = I_x * \bar{f}. \tag{3.16}$$

To increase the efficiency, the original system (3.16) can be replaced by $A * \bar{v} = B * \bar{f}$, where A and B have band structure. We exploit the quasi-inverse technique, and multiply both sides by D_x^{-2}

$$(\alpha D_x^{-2} - I_x^{(2)}) * S_x * \bar{v} = D_x^{-2} * \bar{f}. \tag{3.17}$$

We obtain the 1-D pre-multiplied Galerkin operator $A \equiv (\alpha D_x^{-2} - I_x^{(2)}) * S_x$ (left) and quasi-inverse $B \equiv D_x^{-2}$ (right) which are banded matrices. Since $\tilde{u}_{M-1}$ and $\tilde{u}_M$ are identically

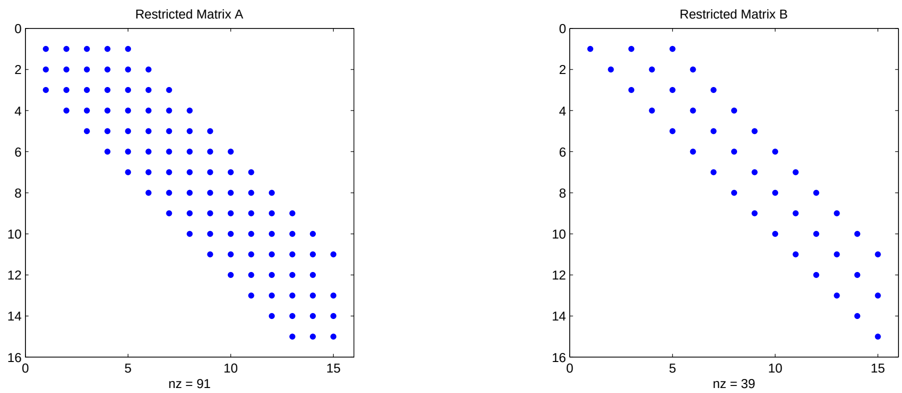

Figure 1: Non-zero (nz) elements of 1-D pre-multiplied restricted Galerkin operator A (left) and quasi-inverse B (right) from Eq. (3.17) with 17 Chebyshev grids.

zero, we can solve the $(M-1)\times(M-1)$ sub-system which is called "restricted system", where we ignore the top two rows and the last two columns of matrices A and B. The non-zero elements of A and B take the form Fig. 1. The cost to solve system of equations is $\mathcal{O}(M)$ operations. After we solve this system of equations, $\bar{v}$ should be converted back to Chebyshev spectral coefficients $\bar{u}$ via the relation (3.13), which requires $\mathcal{O}(M)$ operations since S_x has the special structure. We obtain the approximation solution of $u(x)$ from spectral space to physical space using the forward Chebyshev transform by FFT.

Remark 3.2. We note that for other boundary conditions, we only need identify the corresponding Galerkin basis function and don't need to derive a new spectral Chebyshev differential matrix for each Galerkin basis set by using the transformation matrix. The method for solving elliptic differential equations can easily generalize to two and three dimensional cases.

3.2. 2-D Helmholtz

Consider the 2-D Helmholtz equation

$$\alpha u - \triangle u = f, \quad \text{in } \Omega = I^2,$$

with the homogeneous Robin boundary conditions

$$(a_\pm u + b_\pm u_x)(\pm 1, y) = 0, \ \ (c_\pm u + d_\pm u_y)(x, \pm 1) = 0. \tag{3.18}$$

Let us denote

$$u(x,y) = \sum_{m,n=0}^{M-2,N-2} \tilde{u}_{m,n}\phi_m(x)\phi_n(y),$$

where $\phi_m(x)$ and $\phi_n(y)$ are similar to that in one dimension case. The transformation matrices for each Galerkin basis are the same as they are in one dimension $S_x = E_x^{(0)} + E_x^{(-1)}W_1 + E_x^{(-2)}W_2$ and similarly for S_y. The discrete 2-D Helmholtz system of equations in spectral space is

$$\Big[\alpha(I_x \otimes I_y) - (D_x^2 \otimes I_y + I_x \otimes D_y^2)\Big] * (S_x \otimes S_y) * \bar{v} = (I_x \otimes I_y) * \bar{f}, \tag{3.19}$$

where $\bar{v}$ and $\bar{f}$ are vectors of length $(M-1)\times(N-1)$ formed by the columns of matrices $(\tilde{u}_{m,n})_{m,n=0}^{M-2,N-2}$ and $(\tilde{f}_{m,n})_{m,n=0}^{M-2,N-2}$, respectively. We exploit the quasi-inverse technique similarly to the 1-D case, and multiply both sides by $D_x^{-2} \otimes D_y^{-2}$

$$\Big[\alpha(D_x^{-2} \otimes D_y^{-2}) - (I_x^{(2)} \otimes D_y^{-2} + D_x^{-2} \otimes I_y^{(2)})\Big] * (S_x \otimes S_y) * \bar{v} = (D_x^{-2} \otimes D_y^{-2}) * \bar{f},$$

and employ the Property 3 to obtain

$$\begin{aligned}&\Big[\alpha(D_x^{-2} * S_x \otimes D_y^{-2} * S_y) - (I_x^{(2)} * S_x) \otimes (D_y^{-2} * S_y) - (D_x^{-2} * S_x) \otimes (I_y^{(2)} * S_y)\Big] * \bar{v} \\ =&(D_x^{-2} \otimes D_y^{-2}) * \bar{f}.\end{aligned} \tag{3.20}$$

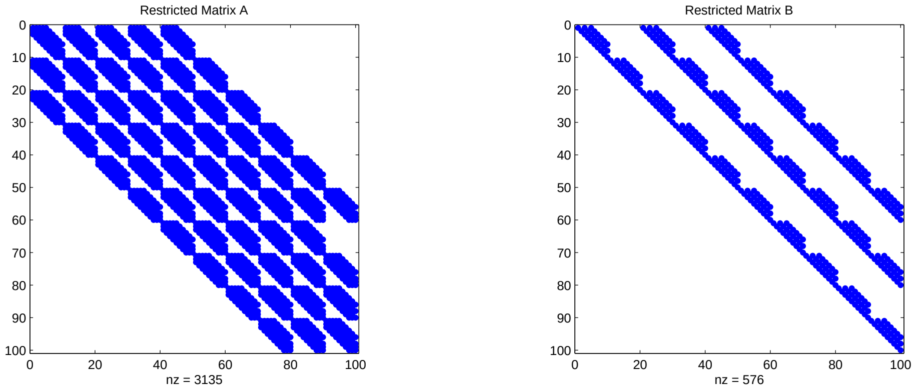

Figure 2: Non-zero (nz) elements of 2-D pre-multiplied restricted Galerkin operator A (left) and quasi-inverse B (right) for the 2-D Helmholtz problem with $12*12$ Chebyshev grids.

From Fig. 2, we can see the strict band structure of 2-D pre-multiplied Galerkin operator

$$A \equiv \alpha(D_x^{-2} * S_x \otimes D_y^{-2} * S_y) - (I_x^{(2)} * S_x) \otimes (D_y^{-2} * S_y) - (D_x^{-2} * S_x) \otimes (I_y^{(2)} * S_y),$$

and quasi-inverse $B \equiv D_x^{-2} \otimes D_y^{-2}$. There are $(M-1)\times(N-1)$ unknowns and the bandwidth grows as $\mathcal{O}(M+N)$, so the cost to solve system of equations is $\mathcal{O}(MN^2+M^2N)$ operations.

3.3. 3-D Helmholtz

The formulation of the 3-D Helmholtz equation with the homogeneous Robin boundary conditions is similar to the 2-D case. We utilize the same Galerkin basis functions and transformation matrices as in the 1-D and 2-D problems. The discrete 3-D Helmholtz system of equations for (3.1) in spectral space is

$$\begin{aligned}&\Big[\alpha(I_x \otimes I_y \otimes I_z) - (D_x^2 \otimes I_y \otimes I_z + I_x \otimes D_y^2 \otimes I_z + I_x \otimes I_y \otimes D_z^2)\Big] * (S_x \otimes S_y \otimes S_z) * \bar{v} \\ =&(I_x \otimes I_y \otimes I_z) * \bar{f}.\end{aligned}$$

We exploit the quasi-inverse technique similarly to the 1-D case, and multiply both sides by $D_x^{-2} \otimes D_y^{-2} \otimes D_z^{-2}$

$$\begin{aligned}&\Big[\alpha(D_x^{-2} \otimes D_y^{-2} \otimes D_z^{-2}) - I_x^{(2)} \otimes D_y^{-2} \otimes D_z^{-2} - D_x^{-2} \otimes I_y^{(2)} \otimes D_z^{-2} - D_x^{-2} \otimes D_y^{-2} \otimes I_z^{(2)}\Big] \\ &* (S_x \otimes S_y \otimes S_z) * \bar{v} = (D_x^{-2} \otimes D_y^{-2} \otimes D_z^{-2}) * \bar{f}.\end{aligned}$$

The original system is replaced by $A * \bar{v} = B * \bar{f}$, where

$$\begin{aligned}A =&\alpha(D_x^{-2} * S_x \otimes D_y^{-2} * S_y \otimes D_z^{-2} * S_z) - (I_x^{(2)} * S_x) \otimes (D_y^{-2} * S_y) \otimes (D_z^{-2} * S_z) \\ &- (D_x^{-2} * S_x) \otimes (I_y^{(2)} * S_y) \otimes (D_z^{-2} * S_z) - (D_x^{-2} * S_x) \otimes (D_y^{-2} * S_y) \otimes (I_z^{(2)} * S_z),\end{aligned}$$

and

$$B = D_x^{-2} \otimes D_y^{-2} \otimes D_z^{-2},$$

which again has a well defined band structure.

Remark 3.3. Since the Dirichlet and Neumann boundary conditions are the special cases of the Robin boundary condition, we can solve the Helmholtz equation with the common three boundary conditions for 1-D, 2-D and 3-D. For nonhomogeneous boundary problems, we always first reduce them to problems with homogeneous boundary conditions by modifying the right-hand side, then solve the homogeneous boundary problems.

Algorithm 3.1. *The Chebyshev spectral method for PDEs using quasi-inverse technique involves the following steps:*

1. *Identify the appropriate Galerkin basis functions to fulfill the boundary conditions;*
2. *For each Galerkin basis in each coordinate, identify the appropriate transformation matrix* S_{x_i}*;*
3. *Evaluate the Chebyshev coefficients* $\{\hat{f}_m\}_{m=0}^M$ *of* $I_M f(x)$ *from* $\{f(x_j)\}_{j=0}^M$ *(backward Chebyshev transform) and evaluate* $\bar{f}$*;*
4. *Discretize the differential equation using the standard Kronecker formalism to obtain* $\mathscr{L}(D) * S_{x_i} * \bar{v} = I_{x_i} * \bar{f}$*;*
5. *Identify the quasi-inverse matrix* B *for the highest order operator in each spatial direction;*
6. *Multiply the system on both sides by* B *to obtain a pre-multiplied system* $A\bar{v} = B\bar{f}$*;*
7. *Solve the system for* $\bar{v}$*;*
8. *Convert from Galerkin basis* $\bar{v}$ *to Chebyshev basis* $\bar{u}$*;*
9. *Evaluate* $u_M(x_j) = \sum_{m=0}^{M} \hat{u}_m T_m(x_j),\ j = 0, 1, \cdots, M$ *(forward Chebyshev transform).*

4. General biharmonic equations

In this section, we generalize the methodology of quasi-inverses to high order problems. Consider the general biharmonic equation

$$\triangle^2 u - \alpha \triangle u + \beta u = f, \quad \text{in } \Omega = I^d, \tag{4.1}$$

with the following two types of boundary conditions

$$u\Big|_{\partial\Omega} = \frac{\partial u}{\partial \mathbf{n}}\Big|_{\partial\Omega} = 0, \tag{4.2}$$

and

$$u\big|_{\partial\Omega} = \frac{\partial^2 u}{\partial \mathbf{n}^2}\bigg|_{\partial\Omega} = 0, \tag{4.3}$$

where $\mathbf{n}$ is the normal vector to $\partial\Omega$ and $d = 1, 2$. (4.2) and (4.3) are named the first and second boundary conditions respectively. Here, we give a uniform treatment to solve the first-kind general biharmonic problem constituted by (4.1) and (4.2) and the second-kind general biharmonic problem constituted by (4.1) and (4.3).

4.1. 1-D General biharmonic equations

Consider the 1-D general biharmonic equation

$$u^{(4)}(x) - \alpha u^{''}(x) + \beta u(x) = f(x), \qquad x \in I, \tag{4.4}$$

with the first boundary conditions $u(\pm 1) = u'(\pm 1) = 0$ and the second boundary conditions $u(\pm 1) = u^{''}(\pm 1) = 0$, respectively. Here, we would like to seek the basis functions of the form

$$\phi_m(x) = T_m(x) + a_m T_{m+2}(x) + b_m T_{m+4}(x).$$

Lemma 4.1. *For the first boundary condition* (4.2)*, we define*

$$a_m = -\frac{2(m+2)}{m+3}, \qquad b_m = \frac{m+1}{m+3}.$$

For the second boundary condition (4.3)*, we define*

$$a_m = -\frac{2(m+2)(15+2m(m+4))}{(m+3)(19+2m(6+m))}, \qquad b_m = \frac{(m+1)(3+2m(m+2))}{(m+3)(19+2m(6+m))}.$$

Then

$$\phi_m(x) = T_m(x) + a_m T_{m+2}(x) + b_m T_{m+4}(x) \tag{4.5}$$

satisfies the first and second boundary conditions respectively.

Proof. Since $T_m(\pm 1) = (\pm 1)^m$ and $T^{''}_m(\pm 1) = \frac{1}{3}(\pm 1)^m m^2(m^2-1)$, the boundary condition $u(\pm 1) = 0$ leads to the following equation for $\{a_m, b_m\}$

$$a_m + b_m = -1. \tag{4.6}$$

The boundary condition $u^{''}(\pm 1) = 0$ leads to the following equation

$$\begin{aligned}&(m^4 + 8m^3 + 23m^2 + 28m + 12)a_m \\ &\quad + (m^4 + 16m^3 + 95m^2 + 248m + 240)b_m = -(m^4 - m^2). \end{aligned}\tag{4.7}$$

By solving the above system (4.6) and (4.7), we obtain $\{a_m, b_m\}$ for the second boundary conditions (4.3). Similarly for the first boundary conditions. $\square$

We identify the transformation matrix for this Galerkin basis (4.5)

$$S_x = E_x^{(0)} + E_x^{(-2)} W_2 + E_x^{(-4)} W_4, \tag{4.8}$$

where W_2 and W_4 are the weight matrices with diagonal entries $\{a_m\}$ and $\{b_m\}$, respectively. We can now write down the matrix form of the discretized equation

$$(D_x^4 - \alpha D_x^2 + \beta I_x) * S_x * \bar{v} = I_x * \bar{f}, \tag{4.9}$$

where $\bar{v}$ has been padded with four zeros at the bottom of the column. We exploit the quasi-inverse technique similarly to the 1-D Helmholtz equation, and multiply both sides by D_x^{-4}

$$(I_x^{(4)} - \alpha D_x^{-4} * D_x^2 + \beta D_x^{-4}) * S_x * \bar{v} = D_x^{-4} * \bar{f}.$$

By employing the Property 2, we obtain

$$I_x^{(4)} * (I_x - \alpha D_x^{-2} + \beta D_x^{-4} * I_x^{(-4)}) * S_x * \bar{v} = D_x^{-4} * \bar{f}. \tag{4.10}$$

The top four rows on both sides are identically zero, so it is trivial to identify appropriate sub-system, shown in Fig. 3. The banded system can be solved in $\mathcal{O}(M)$ operations. The conversion from the Galerkin basis to Chebyshev basis is still $\mathcal{O}(M)$, so the total cost is quasi-optimal.

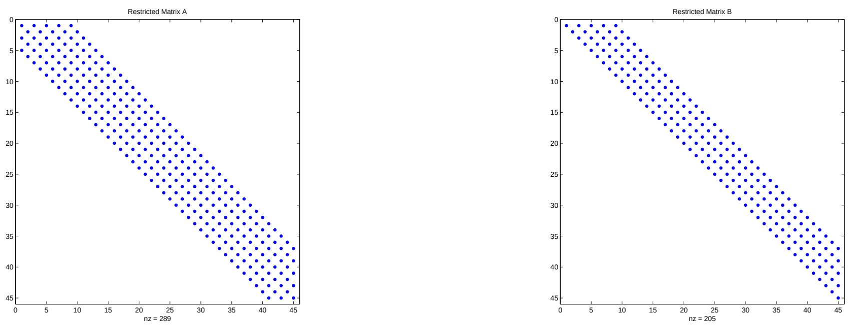

Figure 3: Non-zero (nz) elements of 1-D pre-multiplied restricted Galerkin operator A (left) and quasi-inverse B (right) from Eq. (4.10) with 49 Chebyshev grids.

4.2. 2-D General biharmonic equations

The power of this methodology is its' ready extensibility to higher dimensions and more complicated sets of differential equations. Consider the 2-D general biharmonic equation (4.1) with the first and second boundary conditions respectively. We discretize $u(x,y)$ with the product of two Galerkin basis functions

$$u(x,y) = \sum_{m,n=0}^{M-4,N-4} \tilde{u}_{m,n} \phi_m(x) \phi_n(y),$$

where $\phi_m(x)$ is defined as in the 1-D case and similarly for $\phi_n(y)$. The transformation matrices for each Galerkin basis are the same as they are in one dimension. The discrete 2-D general biharmonic system of equations in spectral space is

$$\begin{aligned}&\Big[D_x^4 \otimes I_y + 2(D_x^2 \otimes D_y^2) + I_x \otimes D_y^4 - \alpha(D_x^2 \otimes I_y + I_x \otimes D_y^2) + \beta(I_x \otimes I_y)\Big] \\ &\quad * (S_x \otimes S_y) * \bar{v} = (I_x \otimes I_y) * \bar{f}. \end{aligned} \tag{4.11}$$

We exploit the quasi-inverse technique similarly to the 2-D Helmholtz equation again, and multiply both sides by $D_x^{-4} \otimes D_y^{-4}$, obtain $A * \bar{v} = B * \bar{f}$, where

$$\begin{aligned} A =& I_x^{(4)} * S_x \otimes D_y^{-4} * S_y + 2(I_x^{(4)} * D_x^{-2} * S_x \otimes I_y^{(4)} * D_y^{-2} * S_y) \\ &+ D_x^{-4} * S_x \otimes I_y^{(4)} * S_y + \beta(D_x^{-4} * S_x \otimes D_y^{-4} * S_y) \\ &- \alpha(I_x^{(4)} * D_x^{-2} * S_x \otimes D_y^{-4} * S_y + D_x^{-4} * S_x \otimes I_y^{(4)} * D_y^{-2} * S_y), \end{aligned} \tag{4.12}$$

and $B = D_x^{-4} \otimes D_y^{-4}$. Because of the structure, it is easy to identify the trivial equations and extract the restricted system, see Fig. 4.

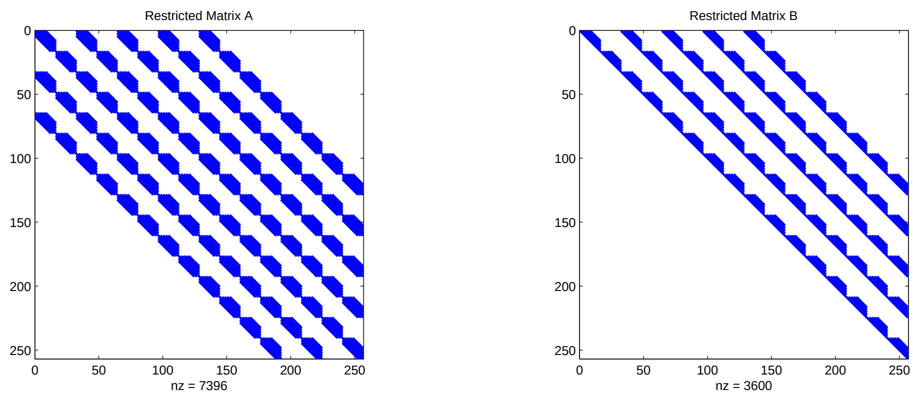

Figure 4: Non-zero (nz) elements of 2-D pre-multiplied restricted Galerkin operator A (left) and quasi-inverse B (right) for the 2-D general biharmonic problem with $20*20$ Chebyshev grids.

Remark 4.1. Because the number of unknowns is the same, the complexity of the solve is roughly the same as that of the 2-D Helmholtz equation, although the bandwidth is slightly wider, it still only grows like $M+N$.

Remark 4.2. In the case of the second-kind general biharmonic problem constituted by (4.1) and (4.3), one can split the governing equation (4.1) into a set of two weakly coupled Poisson equations which can be efficiently solved by employing the proposed method. Although we only study the standard second and fourth order problems, general linear problems can be similarly solved by quasi-inverse methodology.

5. Numerical results

In this section, we give some numerical results obtained by using the algorithms presented in the previous sections. All test codes are implemented in MATLAB and are performed on desktop Dell PC with single core processor. We utilize MATLABs' built-in "sparse" representation for matrices and solve the system of equations via the "backslash" operator. The timing is performed by averaging the time to solve each test problem several separate runs for each number of unknowns.

Table 1: One-dimension Helmholtz equation with three types boundary conditions.

	Dirichlet BC		Neumann BC		Robin BC		
M	$Error_\infty$	$Cond(A)$	$Error_\infty$	$Cond(A)$	$Error_\infty$	$Cond(A)$	$Cond(B)$
8	7.816E-04	8.7	3.983E-04	142.7	1.158E-03	168.3	336
12	2.368E-07	13	9.845E-08	349.6	3.555E-07	399.4	1.72E+3
16	2.297E-11	18	8.084E-12	651.1	3.768E-11	724.8	5.44E+3
20	1.110E-15	22	1.998E-15	1047	1.332E-15	1145	1.33E+4
24	5.551E-16	27	1.998E-15	1536	1.332E-15	1663	2.76E+4

Example 5.1. Consider the following one dimensional Helmholtz equation

$$\alpha u(x) - u^{''}(x) = f(x), \quad x \in I.$$

Given the exact solution under three types boundary conditions. The homogeneous Dirichlet boundary condition and the exact smooth solution

$$u(\pm 1) = 0, \;\; u(x) = \sin(\pi x). \tag{5.1}$$

The homogeneous Neumann boundary condition and the exact smooth solution

$$u'(\pm 1) = 0, \;\; u(x) = \cos(\pi x). \tag{5.2}$$

The homogeneous Robin boundary condition

$$a_\pm u(\pm 1) + b_\pm u'(\pm 1) = 0, \tag{5.3}$$

where $a_\pm = \pi$ and $b_\pm = -1$. Given the following known function

$$f = (\pi^2 + \alpha)(\sin(\pi x) + \cos(\pi x)),$$

the exact solution can be verified to be

$$u(x) = \sin(\pi x) + \cos(\pi x).$$

Table 1 lists the maximum pointwise error of $u - u_M$, condition numbers of matrices A and B using the quasi-inverse technique with $\alpha = 1$ under the three types boundary conditions. Numerical results of this example show that Chebyshev spectral method via quasi-inverse technique converges exponentially under the threex types boundary conditions, because the difference only lies in the different transformation matrices corresponding the Galerkin basis functions. Compared to the condition number of matrix A with Dirichlet boundary condition (Dirichlet BC), those of matrix A with Neumann and Robin BCs are larger.

Example 5.2. Consider the following two dimensional Helmholtz equation

$$\alpha u - \triangle u = f, \quad \text{in } \Omega = I^2.$$

The homogeneous Dirichlet boundary condition and an exact smooth solution are

$$u|_{\partial\Omega} = 0, \quad u(x,y) = \sin(\pi x)\sin(\pi y). \tag{5.4}$$

The homogeneous Neumann boundary condition and an exact smooth solution are

$$\frac{\partial u}{\partial \mathbf{n}}|_{\partial\Omega} = 0, \quad u(x,y) = \cos(\pi x)\cos(\pi y). \tag{5.5}$$

Table 2: Two-dimension Helmholtz equation with two types boundary conditions.

	Dirichlet BC			Neumann BC			
M,N	$Error_\infty$	$Cond(A)$	CPU(s)	$Error_\infty$	$Cond(A)$	CPU(s)	$Cond(B)$
8	1.132E-03	6.20E+3	8.37E-3	3.752E-04	1.03E+4	8.28E-3	1.13E+5
12	4.402E-07	6.97E+4	1.36E-2	1.004E-07	8.00E+4	1.48E-2	2.94E+6
16	4.445E-11	3.90E+5	2.17E-2	8.408E-12	3.55E+5	2.17E-2	2.96E+7
20	1.776E-15	1.48E+6	3.07E-2	3.775E-15	1.15E+6	3.32E-2	1.77E+8
24	8.882E-16	4.42E+6	4.23E-2	4.219E-15	3.06E+6	4.48E-2	7.62E+8

In Table 2, we list the maximum pointwise error of $u - u_{MN}$, condition numbers of matrices A and B and time of solving numerical solutions using the proposed Chebyshev spectral method with $\alpha = 1$ under Dirichlet and Neumann boundary conditions. The results indicate that the spectral accuracy is achieved and the Chebyshev spectral method using quasi-inverse technique is very efficient even for 2-D problems. There is no any difference for the Dirichlet and Neumann boundary conditions, it shows the methodology can be adopted to deal with more complicated boundary problems.

Example 5.3. Consider the 1-D general biharmonic equation with the first boundary conditions:

$$u^{(4)}(x) - \alpha u''(x) + \beta u(x) = f(x), \quad x \in I, \quad u(\pm 1) = u'(\pm 1) = 0, \tag{5.6}$$

with an exact smooth solution $u(x) = \sin^2(4\pi x)$.

This example was used in [10] and [11]. In Table 3, we list the maximum pointwise error of $u - u_M$ and time of solving system of equations $A * \bar{v} = B * \bar{f}$ with two typical choices of α, β. The results indicate that the spectral accuracy is achieved for both α and β are zeros and non-zeros cases. Because the matrices A and B have band structure, we can efficiently solve the system of equations $A * \bar{v} = B * \bar{f}$, and reduce the computing time.

Example 5.4. Consider the 2-D first-kind general biharmonic boundary-value problem (4.1) and (4.2) with an exact smooth solution $u(x,y) = [1+\cos(\pi x)][1+\cos(\pi y)]/\pi^4$.

Table 3: Maximum pointwise error and time with $M+1$ Chebyshev grids.

M	α	β	$Error_\infty$	CPU(s)	α	β	$Error_\infty$	CPU(s)
32	0	0	7.91262E-03	3.77E-5	$2M^2$	M^4	8.78857E-03	7.74E-5
64	0	0	2.08375E-13	3.97E-5	$2M^2$	M^4	2.55351E-15	9.97E-5
128	0	0	5.47562E-13	4.50E-5	$2M^2$	M^4	2.26416E-14	1.50E-4

This problem was solved with $\alpha = 0$, $\beta = 0$ via a spectral collocation method based on integrated Chebyshev polynomials in [8]. For the sake of comparison, we measure the accuracy of a numerical solution via the norm of relative errors of the solution

$$N_e(u) = \sqrt{\frac{\sum\limits_{i,j=0}^{M,N} (u_{i,j}^{(e)} - u_{i,j})^2}{\sum\limits_{i,j=0}^{M,N} (u_{i,j}^{(e)})^2}},$$

where $u_{i,j}^{(e)}$ and $u_{i,j}$ are the exact and computed values of the solution u at point (i,j). In Table 4, we list the relative error $N_e(u)$ and time of solving system of equations $A * \bar{v} = B * \bar{f}$ with two typical choices of α, β. Although the results obtained are slightly less accurate than the proposed integration formulation (PIF) in [8], we can efficiently solve the system for 2-D fourth-order problems because of band structure. We draw the mesh plot of solution of the general biharmonic equation (4.1) with $\alpha = 0$, $\beta = 0$, which is indistinguishable from the exact solution in Fig. 5.

Finally, we compare the actual CPU cost for solving a 2-D Poisson equation and a 2-D biharmonic equation via the proposed algorithms in the previous sections. The two-

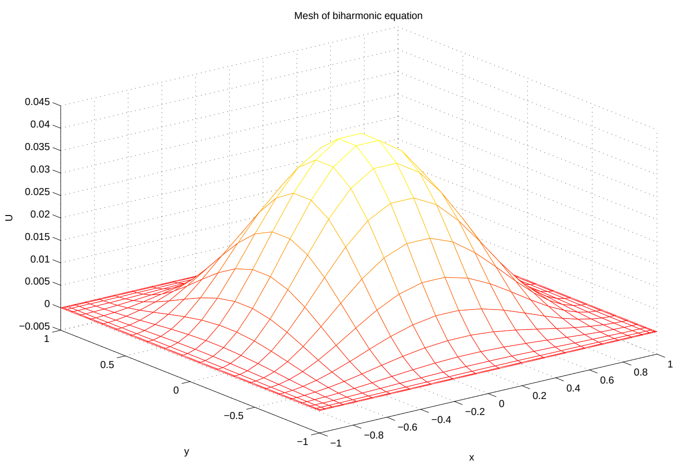

Figure 5: Numerical solution of the 2-D biharmonic problem with $24*24$ Chebyshev grids.

Table 4: Relative error $N_e(u)$ and time for M=N (with $(M+1)*(N+1)$ Chebyshev grids).

$M+1$	α	β	$N_e(u)$	CPU(s)	α	β	$N_e(u)$	CPU(s)
12	0	0	3.57815E-05	7.76E-4	$(M+1)^2$	$(N+1)^4$	6.58325E-05	7.27E-4
16	0	0	3.49722E-09	2.41E-3	$(M+1)^2$	$(N+1)^4$	1.51927E-08	2.62E-3
20	0	0	1.57236E-13	5.14E-3	$(M+1)^2$	$(N+1)^4$	1.17619E-12	5.48E-3
24	0	0	8.85953E-16	9.46E-3	$(M+1)^2$	$(N+1)^4$	4.80108E-16	9.81E-3

dimensional Poisson equation is

$$-\triangle u = 32\pi^2 \sin(4\pi x)\sin(4\pi y), \quad \text{in } \Omega = I^2, \quad u|_{\partial\Omega} = 0, \tag{5.7}$$

with an exact smooth solution $u(x,y) = \sin(4\pi x)\sin(4\pi y)$. The two-dimensional biharmonic equation with the first boundary conditions:

$$\triangle^2 u = f \quad in\ \Omega = I^2, \quad u|_{\partial\Omega} = \frac{\partial u}{\partial \mathbf{n}}|_{\partial\Omega} = 0, \tag{5.8}$$

with an exact smooth solution $u(x,y) = (\sin(2\pi x)\sin(2\pi y))^2$. The two equations were solved by the Legendre-Galerkin method in [9]. In Table 5, we list in the second column the maximum pointwise error of $u-u_{MN}$ and time of solving approximate solution in parentheses of Poisson equation (5.7); in the third column, we list the maximum pointwise error of $u-u_{MN}$ and time of solving approximate solution in parentheses of biharmonic equation (5.8). It is obvious that the approximate solutions converge exponentially to the exact solution. Comparing with the actual time in [9] (the execution time plus the preprocessing time) via Legendre-Galerkin method, the CPU time in seconds via the proposed algorithms is less. It is worth noting that the actual time for solving a 2-D biharmonic equation is 2.5 times of that for solving a 2-D Poisson equation.

Table 5: $Error_\infty$ and CPU time of the Poisson and biharmonic solvers.

M,N	Poisson $Error_\infty$ (CPU)	biharmonic $Error_\infty$ (CPU)
24	6.89445E-06 (0.024)	1.19917E-05 (0.053)
32	4.76170E-11 (0.037)	6.16985E-11 (0.099)
40	3.88578E-15 (0.065)	1.36280E-14 (0.175)
48	2.85882E-15 (0.091)	2.79753E-14 (0.264)

6. Conclusion

We have presented a systematic Chebyshev spectral method using quasi-inverse technique to efficiently solve linear elliptic PDEs. By multiplying the quasi-inverse matrix on the system's both sides, we obtain the system of equations which has band structure, so it can be efficiently solved. We can achieve the same numerical accuracy compared with other methods with less computational cost. The advantages of this methodology are easy to solve the multi-dimensional and more complicated linear elliptic PDEs with a few common boundary conditions. We note that the Chebyshev spectral method via quasi-inverse technique to solve the 2-D general biharmonic equations is very competitive to other existing numerical methods.

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