REFLEXIVE DECOMPOSITIONS FOR SOLVING POISSON EQUATION BY CHEBYSHEV PSEUDOSPECTRAL METHOD

HSIN-CHU CHEN [1], TZYY-LENG HORNG [2], AND YU-HSIANG YANG [2]
[1] DEPT. OF COMPUTER AND INFORMATION SCIENCE, CLARK ATLANTA UNIVERSITY
ATLANTA, GA 30314, USA
[2] DEPT. OF APPLIED MATHEMATICS, FENG-CHIA UNIVERSITY
TAICHUNG, TAIWAN

Abstract. In this paper, we consider the numerical solution to the Poisson equation $\nabla^2 u = f(x,y)$ in the Cartesian domain $\Omega = [-1,1] \otimes [-1,1]$, discretized with the Chebyshev pseudo-spectral method. The boundary conditions are assumed to be Dirichlet on all sides along the domain. The main purpose of this paper is to explore a special reflexivity property inherent in the second-order Chebyshev differentiation matrix and propose a reflexive decomposition scheme for orthogonally decoupling the linear system, derived from the discretization, into independent subsystems. A numerical example is presented to demonstrate the validity and efficiency of the decomposition. In addition to yielding a more efficient algorithm, the proposed scheme also introduces coarse-grain parallelism as a by-product.
AMS (MOS) Subject Classification: 15A04, 15A18.

1 INTRODUCTION

Chebyshev pseudo-spectral methods have long been used to numerically solve partial differential equations [Tref00, Peyr02, MaEs07]. Unlike finite diffence or finite element methods, which generally employ piece-wise polynomials of low order to approximate the solution, this approach usually employs polynomials of much higher-order with unequally spaced grids for non-periodic problems. The advantage of the Chebyshev pseudo-spectral method lies in its ability to achieve much higher accuracy than the other two approaches, given the same number of grid points of the discretized domain or the same dimension of the matrix of coefficients resulting from the discretization. This accuracy advantage, however, does not come without paying prices computationally. The main disadvantage of this approach is mainly due to the fact that the coefficient matrices derived from pseudo-spectral methods are often dense or have a bandwidth very close to the dimension of the matrix. Accordingly, the pseudo-spectral methods cannot really benefit from using banded solvers when direct methods are used to solve the linear systems from the discretization.

In this paper, we resort to a matrix decomposition scheme to decouple the original problem into smaller and independent subproblems by exploring potential special properties of the matrices derived from the Chebyshev pseudo-spectral method. The partial differential equation to be considered is the Poisson equation $\nabla^2 u = f(x,y)$ in the Cartesian domain $\Omega = [-1,1] \otimes [-1,1]$ with homogeneous Dirichlet boundary condition. Without loss of generality we assume $u = 0$ on the boundary, i.e.,

$$\nabla^2 u = f(x,y), (x,y) \in \Omega, \text{ and } u = 0 \text{ on } \partial\Omega. \tag{1}$$

The main focus of this paper is to first explore special properties possesd by the first-order and second-order Chebyshev differentiation matrices. We then, based on the special property of the second-order differentiation matrix, show that the coefficient matrix of the derived linear system exhibits a reflexivity property. This observation enables us to employ reflexive decompositions to decouple the system into independent subsystems, yielding much more efficient numerical computations. This approach can be applied to many other partial differential equations as well, so long as the problem exhibits a reflexivity property, which normally come from some form of reflexive symmetry.

2 CHEBYSHEV DIFFERENTIATION MATRICES AND THEIR SPECIAL PROPERTIES

In this section, we exploit special properties possessed by Chebyshev differentiation matrices and demonstarte how to take advantage of the special property to reduce unnessary numerical computations in solving the Poisson equation. With the Chebyshev pseudo-spectral method, the k^{th} derivative of a function u with respect to x at collocation points $x_j = \cos\left(\frac{j\pi}{N}\right)$, $j = 0, 1, \ldots, N$ can be approximated as

$$\left(\frac{\partial^k u}{\partial x^k}\right) \approx \sum_{j=0}^{N} [D_N^k]_{ij}\ u(x_j), i = 0, 1, \ldots, N$$

where the entries of the collocation derivative matrix D_N, of dimension $N+1$, are [Tref00, Peyr02, MaEs07]

$$[D_N]_{00} = \frac{2N^2+1}{6}, \quad [D_N]_{NN} = -\frac{2N^2+1}{6},$$

$$[D_N]_{jj} = \frac{-x_j}{2(1-x_j^2)}, \quad j = 1, 2, \ldots, N-1$$

$$[D_N]_{ij} = \frac{c_i(-1)^{i+j}}{c_j(x_i - x_j)}, \quad i \neq j, i, j = 0, 1, \ldots, N$$

where $c_i = \left\{ \begin{array}{ll} 2 & \text{for } i = 0 \text{ or } N, \\ 1 & \text{otherwise} \end{array} \right\}$. We shall refer D_N^k to as the k^{th}-order Chebyshev differentiation matrix in this paper. Note that the 1st-order Chebyshev differentiation matrix D_N has the property

$$[D_N]_{ij} = -[D_N]_{N-i,N-j}, \quad i, j = 0, \ldots, N.$$

This property has been observed in [Tref00]. No further exploration of this peoperty, however, has been realized in the literature when the Chebyshev pesudospectral method is employed to solve partial differential equations, to the best of our knowledge. The fact that $[D_N]_{ij} = -[D_N]_{N-i,N-j}$ is equivalent to saying D_N is an anti-centrosymmetric matrix, i.e., $D_N = -J_{N+1}D_N J_{N+1}$ where J_{N+1} is a cross-identity matrix of dimension $N+1$:

$$J_{N+1} = \begin{bmatrix} & & 1 \\ & \ddots & \\ 1 & & \end{bmatrix}.$$

Accordingly, the 2nd-order differentiation matrix, say S, is a centrosymmetric matrix [Andr73a, Andr73b, CaBu76, Weav85]

$$S = D_N^2 = J_{N+1}D_N^2 J_{N+1} = J_{N+1} S J_{N+1}$$

since $J_{N+1}^2 = I_{N+1}$ where I_{N+1} is the identity matrix of dimension $N+1$. Clearly, D_N^k is anti-centrosymmetric for any odd k and is centrosymmetric for and any even k.

When Equation (1) degenerates to a 1D problem, the discretized problem can be solved by the following linear system

$$\tilde{S}\tilde{u} = \tilde{f}, \tilde{S} \in \mathbb{R}^{(N-1)\times(N-1)}, \tilde{u}, \tilde{f} \in \mathbb{R}^{(N-1)}$$

where $\tilde{S}$ is matrix obtained by stripping the first and last rows and columns of S, i.e.,

$$\tilde{S}_{i,j} = S_{i,j} = [D_N^2]_{i,j}, i, j = 1, 2, \ldots, N-1$$

due to Dirichlet boundry conditions. The vector $\tilde{u}$ represents the discretized solution to be found and $\tilde{f}$ denotes the discrete values of $f(x)$ at inner grid points. Note that the stripped matrix $\tilde{S}$ remains a centrosymmetric matrix: $\tilde{S} = J_{N-1}\tilde{S}J_{N-1}$. Now, let us turn to the Poisson equation in two dimensions. Employing a tensor product spectral grid with the same number of Chebyshev points in both directions, Equation (1) may be discretized with lexicographic ordering to yield the following linear system

$$L_N\tilde{u} = \tilde{f}, L_N \in \mathbb{R}^{(N-1)^2\times(N-1)^2}, \tilde{f}, \tilde{u} \in \mathbb{R}^{(N-1)^2} \tag{2}$$

where L_N is the discrete Laplacian operator and may be expressed as [Tref00]

$$L_N = I_{N-1} \otimes \tilde{S} + \tilde{S} \otimes I_{N-1} \tag{3}$$

where $\tilde{S}$ is the same stripped 2nd-order Chebyshev differentiation matrix as in the 1D case and $\otimes$ is the well-known Kronecker product. In the following, we shall denote L_N by K, $I_{N-1} \otimes \tilde{S}$ by K_1 and $\tilde{S} \otimes I_{N-1}$ by K_2 so that Equation (2) becomes

$$K\tilde{u} = \tilde{f}, K = K_1 + K_2. \tag{4}$$

The change of symbols is solely for the sake of notational simplicity for later discussions.

Although the linear system can be solved directly using either an iterative solver or via LU decomposition (or Gaussian eliminations) without difficulties, we shall propose a more efficient way of solving the linear system by taking advantage of a special reflexivity property possessed by the matrix K, before solving the system.

To begin with, let $R = J_{N-1} \otimes I_{N-1}$. For the sake of notational brevity, we shall drop the subscripts associated with I and J in the rest of this section, by assuming all matrix multiplications are conformable. Note that R is a reflection matrix. We show in the following that K has the following property:

$$K = RKR.$$

In other words, we want to show that K is a matrix reflexive with respect to R. First we observe that $I \otimes \tilde{S} = (J \otimes I)(I \otimes \tilde{S})(J \otimes I)$ since

$$(J \otimes I)(I \otimes \tilde{S})(J \otimes I) = \begin{bmatrix} & & I \\ & \iddots & \\ I & & \end{bmatrix} \begin{bmatrix} \tilde{S} & & \\ & \ddots & \\ & & \tilde{S} \end{bmatrix} \begin{bmatrix} & & I \\ & \iddots & \\ I & & \end{bmatrix}$$

$$= \begin{bmatrix} & & I \\ & \iddots & \\ I & & \end{bmatrix} \begin{bmatrix} & & \tilde{S} \\ & \iddots & \\ \tilde{S} & & \end{bmatrix} = \begin{bmatrix} \tilde{S} & & \\ & \ddots & \\ & & \tilde{S} \end{bmatrix} = I \otimes \tilde{S}. \tag{5}$$

Therefore, we have $K_1 = RK_1R$. Next, note that

$$(J \otimes I)(\tilde{S} \otimes I)(J \otimes I) = (J \otimes I)((J\tilde{S}J) \otimes I)(J \otimes I)$$

$$= (J \otimes I)((J \otimes I)(\tilde{S} \otimes I)(J \otimes I))(J \otimes I) = (J \otimes I)^2(\tilde{S} \otimes I)(J \otimes I)^2$$

(6) $$= (I \otimes I)(\tilde{S} \otimes I)(I \otimes I) = \tilde{S} \otimes I$$

where we have used the fact that $\tilde{S} = J\tilde{S}J$ and the equality $(AB) \otimes I = (A \otimes I)(B \otimes I)$. Accordingly, we have $K_2 = RK_2R$. From (5) and (6), we obtain $K = RKR$.

3 REFLEXIVE DECOMPOSITIONS OF K

As seen in the previous section, the matrix K is reflexive with respect to R. The reflexivity property of K enables us to orthogonally decompose K into smaller independent submatrices. The explicit form of the decomposition, however, depends on whether the integer $N-1$ is even or odd. In this paper, we shall consider only the case when $N-1$ is even. Let $N-1 = 2k$ and evenly partition R and K into 2×2 sub-blocks as

(7) $$R = \begin{bmatrix} 0 & R_1 \\ R_1 & 0 \end{bmatrix}, R_1 = J_k \otimes I_{N-1}$$

and

$$K = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}, K_{11} \text{ and } K_{22} \in \mathbb{R}^{k(N-1)\times k(N-1)}.$$

With this partition, the reflexivity property $K = RKR$ implies

(8) $$K_{11} = R_1K_{22}R_1, K_{12} = R_1K_{21}R_1, K_{21} = R_1K_{12}R_1 \text{ and } K_{22} = R_1K_{11}R_1.$$

Now, let X be the following orthogonal matrix:

(9) $$X = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -R_1 \\ R_1 & I \end{bmatrix}.$$

Using the relations in (8), it can easily be shown [ChSa89, Chen94] that the transformation X^TKX decouples K into two independent submatrices as follows.

(10) $$X^TKX = \frac{1}{2} \begin{bmatrix} I & R_1 \\ -R_1 & I \end{bmatrix} \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} I & -R_1 \\ R_1 & I \end{bmatrix} = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}$$

where $D_1 = K_{11} + K_{12}R_1$ and $D_2 = K_{22} - K_{21}R_1$.

In the following, we give the explicit form of the decomposed submatrices D_1 and D_2 in terms of $\tilde{S}$ and its partitioned submatrices. Recall that $K = K_1 + K_2$ where $K_1 = I_{N-1} \otimes \tilde{S}$ and $K_2 = \tilde{S} \otimes I_{N-1}$. It is trivial to see that

(11) $$K_1 = I_{N-1} \otimes \tilde{S} = \begin{bmatrix} I_k \otimes \tilde{S} & 0 \\ 0 & I_k \otimes \tilde{S} \end{bmatrix}$$

since $N-1=2k$ by our assumption. To obtain the partioned form of K_2, we evenly partition $\tilde{S}$ as

$$\tilde{S} = \begin{bmatrix} \tilde{S}_{11} & \tilde{S}_{12} \\ \tilde{S}_{21} & \tilde{S}_{22} \end{bmatrix}, \tilde{S}_{ij} \in \mathbb{R}^{k \times k}.$$

The matrix K_2 can then be expressed as

$$K_2 = \tilde{S} \otimes I_{N-1} = \begin{bmatrix} \tilde{S}_{11} \otimes I_{N-1} & \tilde{S}_{12} \otimes I_{N-1} \\ \tilde{S}_{21} \otimes I_{N-1} & \tilde{S}_{22} \otimes I_{N-1} \end{bmatrix}. \tag{12}$$

From (11) and (12) and the partitioned form of K, we have

$$K_{11} = I_k \otimes \tilde{S} + \tilde{S}_{11} \otimes I_{N-1}, K_{12} = \tilde{S}_{12} \otimes I_{N-1},$$

$$K_{21} = \tilde{S}_{21} \otimes I_{N-1}, \text{ and } K_{22} = I_k \otimes \tilde{S} + \tilde{S}_{22} \otimes I_{N-1}.$$

Accordingly, we have

$$\begin{aligned} D_1 &= (I_k \otimes \tilde{S} + \tilde{S}_{11} \otimes I_{N-1}) + (\tilde{S}_{12} \otimes I_{N-1})R_1 \text{ and} \\ D_2 &= (I_k \otimes \tilde{S} + \tilde{S}_{22} \otimes I_{N-1}) - (\tilde{S}_{21} \otimes I_{N-1})R_1. \end{aligned} \tag{13}$$

As seen from these two decomposed submatrices, the dimension of each of them is only one half of the original matrix. With these two explicit decomposed matrices available, Equation (4) can be solved much more efficiently via the following orthogonal transformation

$$\hat{K}\hat{u} = \hat{f} \text{ where } \hat{K} = X^T K X, \hat{u} = X^T \tilde{u}, \text{ and } \hat{f} = X^T \tilde{f}$$

since this transformation yields the following two smaller and independent subsystems

$$D_i \hat{u}_i = \hat{f}_i, i = 1, 2$$

where $\hat{u}_i$ and $\hat{f}_i$ are simply the evenly partitioned subvectors of $\hat{u}$ and $\hat{f}$, respectively.

4 A NUMERICAL EXAMPLE

To demonstrate the validity of this approach, we present a numerical example of the stripped matrices K obtained from the Poisson equation over a square domain on $[-1,1] \times [-1,1]$, subject to homogeneous Dirichlet boundary conditions with $N = 5$. The matrix K, of dimension 16, is numerically computed to yield

$$K = I_4 \otimes \tilde{S} + \tilde{S} \otimes I_4$$

where

$$\tilde{S} = \begin{bmatrix} -31.5331 & 12.6833 & -3.6944 & 2.2111 \\ 7.3167 & -10.0669 & 5.7889 & -1.9056 \\ -1.9056 & 5.7889 & -10.0669 & 7.3167 \\ 2.2111 & -3.6944 & 12.6833 & -31.5331 \end{bmatrix}.$$

Let

$$R_1 = \begin{bmatrix} & I_4 \\ I_4 & \end{bmatrix}, R = \begin{bmatrix} & R_1 \\ R_1 & \end{bmatrix}, \text{ and } X = \frac{1}{\sqrt{2}} \begin{bmatrix} I_8 & -R_1 \\ R_1 & I_8 \end{bmatrix}.$$

It has already been shown that $K = RKR$ and the transformation $X^T KX$ indeed yields the following decomposed matrix

$$X^T KX = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}$$

where

$$D_1 = \begin{bmatrix} -60.8551 & 12.6833 & -3.6944 & 2.2111 & 8.9889 & 0 & 0 & 0 \\ 7.3167 & -39.3889 & 5.7889 & -1.9056 & 0 & 8.9889 & 0 & 0 \\ -1.9056 & 5.7889 & -39.3889 & 7.3167 & 0 & 0 & 8.9889 & 0 \\ 2.2111 & -3.6944 & 12.6833 & -60.8551 & 0 & 0 & 0 & 8.9889 \\ 5.4111 & 0 & 0 & 0 & -35.8111 & 12.6833 & -3.6944 & 2.2111 \\ 0 & 5.4111 & 0 & 0 & 7.3167 & -14.3449 & 5.7889 & -1.9056 \\ 0 & 0 & 5.4111 & 0 & -1.9056 & 5.7889 & -14.3449 & 7.3167 \\ 0 & 0 & 0 & 5.4111 & 2.2111 & -3.6944 & 12.6833 & -35.8111 \end{bmatrix}$$

and

$$D_2 = \begin{bmatrix} -47.3889 & 12.6833 & -3.6944 & 2.2111 & 9.2223 & 0 & 0 & 0 \\ 7.3167 & -25.9226 & 5.7889 & -1.9056 & 0 & 9.2223 & 0 & 0 \\ -1.9056 & 5.7889 & -25.9226 & 7.3167 & 0 & 0 & 9.2223 & 0 \\ 2.2111 & -3.6944 & 12.6833 & -47.3889 & 0 & 0 & 0 & 9.2223 \\ 16.3777 & 0 & 0 & 0 & -65.2774 & 12.6833 & -3.6944 & 2.2111 \\ 0 & 16.3777 & 0 & 0 & 7.3167 & -43.8111 & 5.7889 & -1.9056 \\ 0 & 0 & 16.3777 & 0 & -1.9056 & 5.7889 & -43.8111 & 7.3167 \\ 0 & 0 & 0 & 16.3777 & 2.2111 & -3.6944 & 12.6833 & -65.2774 \end{bmatrix}.$$

5 CONCLUSIONS

In this paper, we have exploited a special reflexivity property possessed by the second-order Chebyshev differentiation matrix and by the matrix of coefficients in the linear system arising from discretizing the Poisson equation with Dirichlet boundary conditions using Chebyshev pesudo-spectral method. Taking advantage of this special property, we have derived the decomposed submatrices of coefficients explicitly via orthogonal reflexive decompositions. This decomposition enables the original linear system to be solved via the resulting independent linear subsystems to yield parallel and efficient numerical computations. Two numerical examples were presented to demonstrate the decomposition, one for a spectral grid with an odd number of Chebyshev points and the other for an even one. The advantages of our proposed decomposition have also been addressed, which clearly indicates the efficiency of this approach. To close our conclusions, it deserves mentioning that the proposed scheme is applicable to 3D Poisson equation and to a great number of other partial differential equations as well, so long as the physical problems display reflexive symmetry.

6 ACKNOWLEDGEMENTS

The first author Dr. Chen wishes to thank his home institution, Clark Atlanta University, USA for supporting this research area through a sabbatical leave and Feng-Chia University and Tatung University, both in Taiwan for giving him enjoyable environments during his visit to the universities in 2009. The second author Dr. Horng wants to thank the support of Taida Institue of Mathematical Science (TIMS), Taipei, Taiwan and National Center for Theoretical Sciences (NCTS), Hsin-Chu, Taiwan for this work.

REFERENCES

[Andr73a] A.L. Andrew, *Solution of equations involving centrosymmetric matrices*, Technometrics, 15(2) (1973), pp. 405-407.

[Andr73b] A.L. Andrew, *Eigenvectors of certain matrices*, Linear Algebra Appl., 7 (1973), pp. 151-162.

[CaBu76] A. Cantoni and P. Butler, *Eigenvalues and eigenvectors of symmetric centrosymmetric matrices*, Linear Algebra Appl., 13 (1976), pp. 275-288.

[Chen94] H-C. Chen, *Increasing Parallelism in the finite strip formulation: static analysis*, Neural, Parallel & Scientific Computations, 2 (1994), pp. 273-298.

[ChSa89] H-C. Chen and A. Sameh, *A matrix decomposition method for orthotropic elasticity problems*, SIAM J. Matrix Anal. Appl., 10(1) (1989), pp. 39-64.

[Peyr02] R. Peyret, Spectral methods for incompressible viscous problems, Applied Mathematical Sciences, Vol. 148, Ed. Springer-Verlag, New York, 448p., 2002.

[GoLo85] G.H. Golub and C.F. Van Loan, *Matrix Computations*, The Johns Hopkins University Press, Maryland, USA, 1983, 476pp.

[MaEs07] J.d.J. martinez and P.d.T.T. Esperanca, A Chebyshev collocation spectral method for numerical simulation of incompressible flow problems, J. of the Braz. Soc. of mech. Sci. & Eng, Vol. XXIX, No.3 (2007), pp. 317-328.

[Weav85] J.R. Weaver, *Centrosymmetric (cross-symmetric) matrices, their basic properties, eigenvalues, and eigenvectors*, The American Mathematical Monthly, Vol.92, No.10 (1985), pp. 711-717.

[Tref00] Lloyd N. Trefethen, *Spectral Methods in Matlab*, SIAM, University Cith Center, Philadelphia, USA, 2000, 165pp.