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A HIGHLY PARALLEL ALGORITHM FOR SOLVING POISSON EQUATION USING BLOCK DECOMPOSITIONS

HSIN-CHU CHEN

Department of Computer and Information Science, Clark Atlanta University,
Atlanta, GA 30314, USA

ABSTRACT. Poisson equation is frequently encountered in mathematical modeling for scientific and engineering applications. Fast Poisson numerical solvers for 2D and 3D problems are, thus, highly requested for its simulations. In this paper, we consider solving the Poisson equation $\nabla^2 u = f(x,y)$ in the Cartesian domain $\Omega = [-1,1] \otimes [-1,1]$, subject to homogeneous Dirichlet boundary condition, discretized with the Chebyshev pseudo-spectral method. The main purpose of this paper is to propose a two-level block decomposition scheme for decoupling the original linear system obtained from the discretization into independent subsystems. The first level of the block decomposition uses the eigenpairs of the second-order Chebyshev differentiation matrix in one space dimension and the second level of the decomposition exploits a special reflexivity property inherent in this differentiation matrix. The decomposition not only yields a more efficient algorithm but introduces high-degree coarse-grain parallelism. This approach can also be applied to Laplace eigenvalue problem discretized with the Chebyshev pseudo-spectral method as well, subject to the same boundary conditions.

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1. INTRODUCTION

In this paper, we consider the numerical solution to the Poisson equation $\nabla^2 u = f(x,y)$ in the Cartesian domain $\Omega = [-1,1] \otimes [-1,1]$ with homogeneous Dirichlet boundary condition. Without loss of generality we assume $u = 0$ on the boundary, i.e.,

$$\nabla^2 u = f(x,y), (x,y) \in \Omega, \text{ and } u = 0 \text{ on } \partial\Omega, \tag{1.1}$$

since the solution can be obtained by modifying the right-hand side of the linear system using the known boundary values without changing its coefficent matrix. We present a highly parallel block decomposition scheme for decoupling the coefficient matrix of the linear system derived from the discretization of this equation using the Chebyshev pseudo-spectral method. Chebyshev pseudo-spectral methods have long been used to numerically solve partial differential equations [12, 11, 10]. 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

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of much higher-order with unequally spaced grids for non-periodic problems. The advantage of the spectral method lies in its ability to achieve much higher accuracy than the other two approaches, given the same number of grid points in the discretized domain, or the same dimension of the matrix of coefficients resulting from the discretization. However, this accuracy advantage does not come without paying prices computationally. The trade-off lies in the fact that the coefficient matrices derived from the finite difference or finite element methods are usually narrow-banded, whereas those yielded by the spectral methods are either dense or have a bandwidth very close to the dimension of the matrix. Accordingly, the spectral methods cannot really benefit from using banded solvers when direct methods are used to solve the linear systems from the discretization. This is rather a disadvantage of the spectral methods in terms of computational complexity. Other approaches that can take advantage of the special structure and special properties of the coefficient matrix, therefore, deserves further exploitation. In this paper, a two-level block decomposition scheme is presented to achieve this goal. We develop the explicit form of the decomposed subsystems and presebt a numerical example to illustrate its validity and simplicity.

2. CHEBYSHEV COLLOCATION MATHOD

In this section, we briefly describe the Chebyshev collocation method for solving the Poisson equation in two dimensions. We assume that the problem is discretized with a tensor product grid (x_i, y_j), $0 \le i, j \le N$, where x_i and y_j are the Chebyshev points in x and y direction, respectively. Let D_N, indexed from 0 to N, be the $(N+1)*(N+1)$ Chebyshev spectral differentiation matrix associated with the x direction. The entries of D_N are given as [12, 11, 10]

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

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

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

where $c_i = \left\{ \begin{array}{ll} 2 & \text{for } i = 0 \text{ or } N, \\ 1 & \text{otherwise} \end{array} \right\}$. Now, let A be the stripped matrix of D_N^2 by removing the first and last rows and columns of D_N^2. In other words,

$$A_{ij} = (D_N^2)_{ij}, i, j = 1, 2, \cdots, N-1.$$

With the grid just described, the Chebyshev collocation method yields, after removing the boundary nodes whose values are already known from the system, the following linear system

$$Ku = f, K = I_{N-1} \otimes A + A \otimes I_{N-1} \tag{2.1}$$

where I is the identity matrix of dimension $N-1$.

3. TWO-LEVEL DECOMPOSITIONS

Many solution schemes can be employed to solve (2.1), including Gaussian eliminations, Gauss-Seidel iterations, alternating direction implicit (ADI) iterations, and matrix diagonalizations [6, 7, 8]. In this paper, the matrix diagonalization method will be employed first to decompose the matrix K into a block diagonal matrix consisting of $N-1$ diagonal blocks. Each diagonal block will then be further decomposed into two smaller diagonal sub-blocks using reflexive decompositions, yielding a total of $2(N-1)$ diagonal sub-blocks. This two-step deomposition scheme allows for the linear system (2.1) to be decoupled into $2(N-1)$ linear subsystems which can then be solved in parallel with course-grain parallelism using multiprocessors or networked computers. The explicit forms of the decomposed matrices are derived at the end of this section.

3.1. **Level-1 Decomposition: Block Diagonalization.** In this subsection, we address the decomposition of the matrix K into $N-1$ diagonal blocks using a matrix representation, although the diagonalization approach has long been presented and used [9, 7, 5, 8]. To begin with, let Q_A be such a matrix that the similarity transformation $Q_A^{-1}AQ_A$ diagonalizes A into Λ:

$$Q_A^{-1}AQ_A = \Lambda$$

A natural choice of Q_A is to have its columns formed from the eigenvectors of A so that Λ is a diagonal matrix that consists of the eigenvalues of A. Now let $Q = I_{N-1} \otimes Q_A$ and split the coefficient matrix K in (2.1) into two parts: $K_1 = I_{N-1} \otimes A$ and $\mathrm{K}_2 = \mathrm{A} \otimes \mathrm{I}_{\mathrm{N}-1}$. By applying the similarity transformation$Q^{-1}KQ$, we have the transformed matrix

$$\tilde{K} = \tilde{K}_1 + \tilde{K}_2; \tilde{K} = Q^{-1}KQ, \tilde{K}_1 = Q^{-1}K_1Q, \tilde{K}_2 = Q^{-1}K_2Q$$

where

$$Q^{-1} = I_{N-1} \otimes Q_A^{-1}.$$

We now show that the transformed matrix $\tilde{K}$ can be permuted to yield a block diagonal matrix. First note that both $\tilde{K}_1$ and $\tilde{K}_3$ are diagonal matrices and $\tilde{K}_2$ is a diagonal block matrix since

$$\tilde{K}_1 = Q^{-1}K_1Q = (I_{N-1} \otimes Q_A^{-1})(I_{N-1} \otimes A)(I_{N-1} \otimes Q_A) = I_{N-1} \otimes (Q_A^{-1}AQ_A) = I_{N-1} \otimes \Lambda,$$

and

$$\tilde{K}_2 = Q^{-1}K_2Q = (I_{N-1} \otimes Q_A^{-1})(A \otimes I_{N-1})(I_{N-1} \otimes Q_A) = A \otimes I_{N-1}.$$

Accordingly,

$$\tilde{K} = Q^{-1}KQ = I_{N-1} \otimes \Lambda + A \otimes I_{N-1}. \tag{3.1}$$

Let a_{ij} be the $(i,j)^{th}$ element of A, $i,j = 1,2,\cdots,N-1$. In its matrix form, $\tilde{K}$ can be expressed as

$$\tilde{K} = \begin{bmatrix} a_{11}I + \Lambda & a_{12}I & \cdots & a_{1p}I \\ a_{21}I & a_{22}I + \Lambda & \cdots & a_{2p}I \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1}I & a_{p2}I & \cdots & a_{pp}I + \Lambda \end{bmatrix}$$

where $p = N-1$. Apparently, $\tilde{K}$ is also a diagonal block matrix because both I and Λ are diagonal matrices. The diagonal block matrx $\tilde{K}$ can be rearranged to yield a block diagonal matrix $\hat{K}$:

$$\hat{K} = \begin{bmatrix} \hat{K}_1 & 0 & \cdots & 0 \\ 0 & \hat{K}_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \hat{K}_p \end{bmatrix}$$

via appropriate permutations of rows and columns. Let $\tilde{K}_{ij}$ be the $(i,j)^{th}$ block of $\tilde{K}$ and P be such a permutation matrix that the transformation $P^T\tilde{K}P$ rearranges the entries of $\tilde{K}$ in such a way that

$$\hat{K}_l(i,j) = \tilde{K}_{i,j}(l), i,j = 1,2,...,p$$

where $\hat{K}_l(i,j)$ is the $(i,j)^{th}$ element of $\hat{K}_l$ and $\tilde{K}_{i,j}(l)$ is the l^{th} diagonal element of $\tilde{K}_{i,j}$. Then we have

$$P^T\tilde{K}P = \hat{K} = \hat{K}_1 \oplus \hat{K}_2 \oplus \cdots \oplus \hat{K}_p, \text{ where } \hat{K}_l = A + \lambda_l I, l = 1,2,\cdots,p. \tag{3.2}$$

3.2. **Level-2 Decomposition: Reflexive Decomposition.** In this subsection, we propose to further decompose each of the diagonal blocks $\hat{K}_l$ into two smaller sub-blocks by employing another decomposition technique called the reflexive decomposition [3, 4]. First, we observe that both A and I satisfy the reflexivity property with respect to R with R being the cross identity matrix of dimension $N-1$, J_{N-1}:

$$A = RAR, I = RIR, \text{ where } \mathrm{R} = \mathrm{J_{N-1}} = \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}.$$

In fact, both A and I are centrosymmetric matrices [1, 2], which are special cases of reflexive matrices. Accordingly, $\hat{K}_l$ satisfy the reflexivity property $\hat{K}_l = R\hat{K}_lR, l = 1,2,\cdots,p$. Therefore, each of them can be decomposed into two block diagonal submatrices of almost equal size, depending on whether the size of $\hat{K}_l$ is even or odd.

The decompositions can be done through orthogonal transformations which has been shown in [4]. Here we just present the results.

First consider the case when $N-1$ is even. Assume $N-1 = 2k$ for some $k > 0$, and A is evenly partitioned into 2×2 sub-blocks: $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$. Taking the advantage of the reflexivity property of $\hat{K}_l$ by applying the orthogonal transformation $X_A^T \hat{K}_l X_A$ to $\hat{K}_l$ where $X_A = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -R_1 \\ R_1 & I \end{bmatrix}$ with $R_1 = J_k$, one can easily decompose $\hat{K}_l$ into two decoupled diagonal subblocks:

$$D_l = X_A^T \hat{K}_l X_A = X_A^T (A + \lambda_l I) X = X_A^T A X_A + \lambda_l I = \begin{bmatrix} D_{l1} & 0 \\ 0 & D_{l2} \end{bmatrix} \tag{3.3}$$

where

$$D_{l1} = A_{11} + A_{12} R_1 + \lambda_l I_k \text{ and } D_{l2} = A_{22} - A_{21} R_1 + \lambda_l I_k.$$

In the case when $N-1$ is odd, say $N-1 = 2k+1, k > 0$, we consistently partition A and R as

$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & a_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}, R = \begin{bmatrix} & & R_1 \\ & 1 & \\ R_1 & & \end{bmatrix}, R_1 = J_k.$$

By taking the transformation matrix X_A to be $X_A = \frac{1}{\sqrt{2}} \begin{bmatrix} I & 0 & -R_1 \\ 0 & \sqrt{2} I_{N-1} & 0 \\ R_1 & 0 & I \end{bmatrix}$, the matrix $\hat{K}_l$ can be decoupled via the orthogonal transformation $X_A^T \hat{K}_l X_A$ as

$$D_l = X_A^T \hat{K}_l X_A = X_A^T (A + \lambda_l I) X_A = X_A^T A X_A + \lambda_l I = \begin{bmatrix} D_{l1} & 0 \\ 0 & D_{l2} \end{bmatrix}$$

where

$$D_{l1} = \begin{bmatrix} A_{11} + A_{13} R_1 & \sqrt{2} A_{12} \\ \sqrt{2} A_{21} & a_{22} \end{bmatrix} + \lambda_l I_{k+1} \text{ and } D_{l2} = (A_{33} - A_{31} R_1) + \lambda_l I_k.$$

In short, let $X = I_p \otimes X_A = X_A \oplus X_A \oplus \ldots \oplus X_A$. The orthogonal transformation $X^T \hat{K} X$ yields

$$D = D_1 \oplus D_2 \oplus \ldots \oplus D_p = (D_{11} \oplus D_{12}) \oplus (D_{21} \oplus D_{22}) \oplus \ldots (D_{p1} \oplus D_{p2}),$$

which apparently consists of $2p$ independent diagonal blocks.

3.3. **Computational Considerations.** Recall that the original linear system to be solved is

$$Ku = f, K = I_p \otimes A + A \otimes I_p, p = N - 1$$

where I_p is the identity matrix of dimension p and the matrix K is of dimension p^2. Instead of solving this system directly, we shall solve the following transformed linear system which consists of $2p$ independent subsystem, each of dimension $\frac{p}{2}$:

$$Dv = g, D = (D_{11} \oplus D_{12}) \oplus (D_{21} \oplus D_{22}) \oplus \dots (D_{p1} \oplus D_{p2}).$$

Given the availability of the eigenpairs of A, these independent subsystems are obtained, in theory, via the stages shown below.

1. Transform $Ku = f$ to $\tilde{K}\tilde{u} = \tilde{g}$, $\tilde{K} = Q^{-1}KQ$, $\tilde{u} = Q^{-1}u$, $\tilde{f} = Q^{-1}f$.
2. Transform $\tilde{K}\tilde{u} = \tilde{g}$ to $\hat{K}\hat{u} = \hat{g}$, $\hat{K} = P^T\tilde{K}P$, $\hat{u} = P^T\tilde{u}$, $\hat{f} = P^T\tilde{f}$.
3. Transform $\hat{K}\hat{u} = \hat{g}$ to $Dv = g$, $D = X^T\hat{K}X$, $v = X^T\hat{u}$, $g = X^T\hat{f}$.

In practice, it is important to note that the decomposed form of D is explicitly known and, therefore, the actual decompositions from K to $\tilde{K}$, from $\tilde{K}$ to $\hat{K}$, and from $\hat{K}$ to D are not necessary. Furthermore, the diagonal blocks of D can be obtained without any matrix-matrix multiplications.

To obtain g, we need to transform f to $\tilde{f}$ first, which involves solving the linear system $Q\tilde{f} = f$. It is crucial to note that $Q, Q = I_p \otimes Q_A$, is a block diagonal matrix and, therefore, $\tilde{f}$ can be obtained by solving p independent linear systems of size p, instead of solving the whole linear system, which is of size p^2. This step can be performed in parallel with large granularity. The matrix Q_A, consisting of the eigenvectors of A, is in general not known explicitly and, thus, has to be computed from A. Fortunately, A is only of dimension p. Once $\tilde{f}$ is ready, $\hat{f}$ and g can be obtained easily. Note that $\hat{f}$ is simply a permuted version of $\tilde{f}$ and $g = X^T\hat{f}$ involves no matrix-vector multiplication because of the specil form of X. With D and g available, the linear system $Dv = g$ can be solved for v in parallel, using $2p$ processors, one for each subsystem. The solution u to the original system can then be retrieved from v without any difficulty. To end this section, Note that this two-level decomposition is a similarity transformation and therefore, all eigenvalues of the original matrix K are preserved in matrix D. Obtaing eigenvalues from D is far more efficient than from K.

4. NUMERICAL EXAMPLE

To illustrate this approach, we present a numerical example for the decomposition of the coefficient matrix K derived from the Poisson equation over a square domain on $[-1, 1] \times [-1, 1]$, subject to homogeneous Dirichlet boundary conditions on a square grid with $N_x = N_y = 5$. The numerical results presented in this section were obtained using Octave. By excluding the grid points on the boundary and using the lexicographic ordering to number the internal nodes [12], the matrix K, of dimension 16, can be numerically computed to yield

$$K = I_4 \otimes A + A \otimes I_4$$

where

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

Let the columns of Q_A be the eigenvectors of A, of dimension 4, and P^T be the following permutation matrix of dimension 16

$$P^T(k,l) = \begin{cases} 1 & \text{for } k = j + (i-1) * 4, l = i + (j-1) * 4, 1 \leq i, j \leq 4 \\ 0 & \text{otherwise.} \end{cases}$$

From the Level-1 decomposition presented in Section 3,

$$P^T \tilde{K} P = \hat{K} = P^T Q^{-1} K Q P = \hat{K}_1 \oplus \hat{K}_2 \oplus \hat{K}_3 \oplus \hat{K}_4, Q = I_4 \otimes Q_A,$$

we easily obtain the decoupled diagonal blocks $\hat{K}_l$ without the need of any matrix multiplications once the eigenvalues of A are available:

$$\hat{K}_l = A + \lambda_l = \begin{bmatrix} -31.5331 + \lambda_l & 12.6833 & -3.6944 & 2.2111 \\ 7.3167 & -10.0669 + \lambda_l & 5.7889 & -1.9056 \\ -1.9056 & 5.7889 & -10.0669 + \lambda_l & 7.3167 \\ 2.2111 & -3.6944 & 12.6833 & -31.5331 + \lambda_l \end{bmatrix},$$

$1 \leq l \leq 4$, where $\lambda = \{-40.00, -31.13, -9.600, -2.467\}$, the eigenvalues of A corresponding to Q_A.

The numerical values of $\hat{K}_l$ clearly indicate that each $\hat{K}_l$ is reflexive with respect to $R = J_4$. Now, applying the Level-2 decomposiiton to each $\hat{K}_l$ by taking $X = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -J_2 \\ J_2 & I \end{bmatrix}$ yields

$$D_1 = X^T \hat{K}_1 X = \begin{bmatrix} -69.32 & 8.99 & & \\ 5.41 & -44.28 & & \\ & & -55.86 & 9.22 \\ & & 16.38 & -73.74 \end{bmatrix},$$

$$D_2 = X^T \hat{K}_2 X = \begin{bmatrix} -60.46 & 8.99 & & \\ 5.41 & -35.41 & & \\ & & -46.99 & 9.22 \\ & & 16.38 & -64.88 \end{bmatrix},$$

$$D_3 = X^T \hat{K}_3 X = \begin{bmatrix} -38.92 & 8.99 & & \\ 5.41 & -11.88 & & \\ & & -25.46 & 9.22 \\ & & 16.38 & -43.34 \end{bmatrix},$$

$$D_4 = X^T \hat{K}_4 X = \begin{bmatrix} -31.79 & 8.99 & & \\ 5.41 & -6.74 & & \\ & & -18.32 & 9.22 \\ & & 16.38 & -36.21 \end{bmatrix}$$

where, for simplicity, we have rounded off the numbers after the last digit shown. The unshown entries in the matrices are 0. Apparently, each $\hat{K}_l$ has been further decomposed into two independent diagonal blocks, yielding a total of eight independent diagonal blocks from the original matrix K. Note that the decomposed matrices $D_l, 1 \le l \le 4$, can be obtained directly from A and λ_l using Eq.(3.3) without the need of computing $\hat{K}_l$.

5. **CONCLUSIONS**

In this paper, we have presented a two-level block decomposition scheme for the numerical solution to the Poisson equation in a rectangular domain subject to Dirichlet boundary conditions, which is discretized by the Chebyshev pseudo-spectral method. The first level of the decomposition schem employs the eigenpairs of the 1D second-order Chebyshev differentiation matrix to reduce a 2D problem into independent 1D subproblems, after a proper permutation of the decoupled coefficient matrix. For a computational grid with $N+1$ grid points in each direction, this level of decomposition yields $N-1$ independent subproblems, excluding the boundary points. In the second-level decomposition, each of the subproblem is then further decomposed into two independent subproblems by taking advantage of a special reflexivity property inherent in the decomposed submatrix, yielding a total of $2(N-1)$ independent subproblems.

The explicit form of the coefficient matrix of each independent subproblem, decoupled by the two-level block decomposition, has also been derived and a numerical example presented to illustrate its validity and simplicity. This block decomposition scheme leads naturally to a highly parallel numerical algorithm for solving the problem under consideration, since all subproblems can be solved in parallel using multiprocessors. Finally, It deserves mentioning that the first-level decomposition is a similarity transformation and the second-level decomposition is an orthogonal transformation. Therefore, all eigenvalues of the original 2D problem are preserved in the decomposed submatrices and can be obtained from them directly and much more efficiently, in addition to the computational benefit that can be achieved from the large-grain parallelism induced by the decomposition.

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