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Incomplete double-cone factorizations of centrosymmetric matrices arising in spectral methods

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Abstract
We develop structure-preserving incomplete LU type factorizations for preconditioning centrosymmetric matrices and use them to numerically solve centrosymmetric and nearly centrosymmetric linear systems arising from spectral methods for partial differential equations. Our algorithm builds in part on direct solution techniques previously developed for this type of linear systems, featuring double-cone factorizations. We illustrate our findings on discretizations of model problems involving the Poisson, diffusion, Helmholtz, and biharmonic equations in one, two, and three dimensions.

Keywords Numerical solution of linear systems · Centrosymmetric matrix · Spectral differentiation · Double cone · Preconditioning · Incomplete LU factorization

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1 Introduction

A matrix $\mathcal{A} = (a_{ij}) \in \mathbb{R}^{n\times n}$ is *centrosymmetric* if it is symmetric about its center:

$$a_{i,j} = a_{n+1-i,n+1-j}, \qquad 1 \le i, j \le n. \tag{1}$$

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It has been shown [1] that $\mathcal{A} \in \mathbb{R}^{n\times n}$ is centrosymmetric if and only if $J\mathcal{A}\mathcal{J} = \mathcal{A}$, where $J \in \mathbb{R}^{n\times n}$ is a matrix with ones along the antidiagonal and zeros elsewhere

$$J = \begin{bmatrix} & & 1 \\ & \ddots & \\ 1 & & \end{bmatrix} \in \mathbb{R}^{n\times n}.$$

The matrix J is called a flip matrix or the reverse identity matrix.

The family of centrosymmetric matrices includes a number of important types that arise in a variety of applications, e.g., in the numerical solution of partial differential equations (PDEs), signal processing, and Markov processes [2–4]. Two instances of centrosymmetric matrices are symmetric Toeplitz and symmetric circulant matrices. Numerical methods for solving problems involving such matrices have been extensively explored in the literature; see [5, 6], for example. Various preconditioners have been proposed for solving symmetric systems involving Toeplitz matrices; see [7–10]. Ng et al. [11] proposed a recursive-based preconditioned conjugate gradient method for symmetric positive definite ill-conditioned Toeplitz systems. Fast algorithms for centrosymmetric Toeplitz-plus-Hankel matrices are discussed in [12–14]. Notice that if T is symmetric Toeplitz, then JT is a centosymmetric Hankel matrix. Tian and Gu [15] introduced economical iterative methods for centrosymmetric M-matrices.

An important early observation related to the block structure of centrosymmetric matrices is the following similarity transformation [1]. If $\mathcal{A} \in \mathbb{R}^{n\times n}$ is centrosymmetric, where $n = 2k$, then it has the form

$$\mathcal{A} = \begin{bmatrix} A & JCJ \\ C & JAJ \end{bmatrix},$$

where $A, C, J \in \mathbb{R}^{k\times k}$. This matrix can be block-diagonalized via an orthogonal similarity transformation

$$\mathcal{A} = \mathcal{U} \begin{bmatrix} A + JC & 0 \\ 0 & A - JC \end{bmatrix} \mathcal{U}^T, \qquad \mathcal{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} I & I \\ J & -J \end{bmatrix}, \tag{2}$$

where $I \in \mathbb{R}^{k\times k}$. Note that since $\mathcal{U}$ is orthogonal, the spectrum of $\mathcal{A}$ consists of the union of the spectra of $A \pm JC$. The case of the dimension n being an odd number is slightly more involved notation-wise but is otherwise analogous.

The set $\mathcal{C}_n$ of $n \times n$ centrosymmetric matrices is an algebra: If $\mathcal{A}, \mathcal{B} \in \mathcal{C}_n$ and $a \in \mathbb{R}$, then $\mathcal{A} + \mathcal{B}$, $\mathcal{A}\mathcal{B}$, $a\mathcal{A} \in \mathcal{C}_n$. If $\mathcal{A} \in \mathcal{C}_n$, so is $\mathcal{A}^T$. If $\mathcal{A} \in \mathcal{C}_n$ is invertible, then $\mathcal{A}^{-1} \in \mathcal{C}_n$, and each diagonal block in (2) is invertible. Suppose n is even, then $\mathcal{A} \in \mathcal{C}_n$ is Hermitian (resp. skew-Hermitian, normal, positive definite) if and only if $A+JC$ and $A - JC$ are Hermitian (resp. skew-Hermitian, normal, positive definite). Analogous results hold when n is odd. See [1, 16, 17] for various properties of centroymmetric matrices. Also see [18–20] for attributes of structured matrices.

The development of direct solvers for centrosymmetric linear systems has led to computational gains. Early work was published by Andrew [21] almost five decades ago. Instead of solving the original centrosymmetric system, he solved two linear systems half the size, which require only about half the total storage and a quarter of the total computational time. See [22, 23] for additional details. Recently, a new factorization for centrosymmetric matrices was introduced by Burnik [24]. He proposed an algorithm for factoring a centrosymmetric matrix as a product of a centrosymmetric orthogonal matrix Q and a centrosymmetric matrix X with a special structure called *double-cone*. Steele et al. [25] introduced a different algorithm for computing the QX factorization based on the similarity transformation (2). Perturbation analysis and conditions for uniqueness of the QX factorization are derived by Lv and Zheng [26].

Of particular interest to us are centrosymmetric matrices that arise in spectral methods for solving PDEs. The latter are known to efficiently solve problems involving regular geometry with spectral accuracy, provided the solution is smooth. They require fewer degrees of freedom to achieve a given accuracy compared to other methods such as finite-difference approximations [27, 28]. The matrices come in a few distinct flavors, depending on the number of space dimensions and the specific PDE. In this paper, we consider the Poisson, diffusion, Helmholtz, and biharmonic equations in one, two, and three dimensions. As described later, some of the corresponding linear systems are dense while others are sparse. In some dense cases, certain additive components are sparse. Thus, there is a rich structure here, which may be exploited to design fast solvers.

We note that matrices arising from spectral methods are typically not very large, thanks to the extreme accuracy that those methods offer. And yet, preconditioned iterative solvers are still potentially useful, especially for three-dimensional problems, for a variety of reasons related to the typical advantages that iterative methods offer, for example, the ability of those methods to compute a solution to a low accuracy and the ability to exploit the availability of a good initial guess. Matrices arising in spectral methods are typically ill-conditioned, and this poses a challenge for any type of numerical solvers.

We derive incomplete LU type factorizations that preserve the structure and take advantage of a fast matrix–vector product proposed by Melman [29] and Fassbender and Ikramov [30]. We then apply preconditioned iterative solvers for various spectral differentiation matrices. For the Poisson and Helmholtz equations, we apply preconditioners defined by incomplete double-cone factors of the matrices arising from Chebyshev and Legendre collocation methods. The biharmonic equation produces a dense matrix due to the mixed derivatives, and we approximate this part by a finite-difference scheme based on collocation points and combine it with the other (sparse) parts of the matrix. We then use the incomplete factorization of this approximation as a preconditioner for the linear system. When the matrix is symmetric positive definite, we apply preconditioned conjugate gradient (PCG); otherwise, we apply a generalized minimum residual (GMRES). Our proposed preconditioners show promise in terms of speed of convergence and overall computational cost. We explore the feasibility of these techniques on an extensive set of centrosymmetric and nearly centrosymmetric matrices arising from the important class of spectral methods for the numerical solution of PDEs.

An outline of the remainder of this paper follows. In Sect. 2, we discuss centrosymmetric matrices that arise in spectral collocation methods. In Sect. 3, the double-cone factorization is described, and we explain how to apply it to derive an incomplete LU or Cholesky factorization. GMRES (PCG in SPD cases) with proposed preconditioners are applied to diffusion and variable-coefficient biharmonic equations. Section 4 offers comprehensive numerical experiments that validate our claims. Finally, in Sect. 5, we draw some conclusions.

2 Spectral differentiation matrices

Consider the linear boundary value problem

$$\mathcal{L}u = f \quad \text{in} \quad (-1, 1), \tag{3}$$

with homogeneous Dirichlet boundary conditions. Let P_N^0 denote the space of polynomials of degree at most N vanishing at ± 1. Let $x_0, \ldots, x_N$ denote Chebyshev Gauss-Lobatto nodes with $x_0 = 1$, $x_N = -1$ and x_j descending zeros of $T_N'(x)$, where $1 \leq j \leq N-1$ and T_N is the Nth Chebyshev polynomial. Spectral collocation, also known as pseudospectral approximation, seeks a polynomial $u_N \in P_N^0$ such that the approximate solution u_N of (3) satisfies the equation exactly at the collocation points.

Given any set of distinct collocation points $\{x_j\}_{j=0}^N$ on $[-1, 1]$, let ℓ_j be the Lagrange interpolant, a polynomial of degree N, so that $\ell_j(x_k) = \delta_{jk}$. Then, u_N can be expressed as

$$u_N(x) = \sum_{j=1}^{N-1} u_N(x_j)\ell_j(x). \tag{4}$$

Substituting this in (3) gives the collocation equations $\mathcal{L}u_N(x_j) = f(x_j)$, for $1 \leq j \leq N-1$. Differentiating (4) m times leads to

$$u_N^{(m)}(x_k) = \sum_{j=1}^{N-1} u_N(x_j)\ell_j^{(m)}(x_k), \quad 1 \leq k \leq N-1.$$

The first-order spectral differentiation matrix $D \in \mathbb{R}^{(N+1)\times(N+1)}$ has entries

$$D_{jk} = \frac{d\ell_k(x_j)}{dx}, \qquad 0 \leq j, k \leq N.$$

Then, $D^{(m)} = DD\cdots D = D^m$, for $m \geq 1$, where

$$D_{jk}^{(m)} = \frac{d^m \ell_k(x_j)}{dx^m}, \qquad 0 \leq j, k \leq N,$$

is the mth spectral differentiation matrix; see Theorem 3.10 [28]. For Chebyshev collocation, explicit formulas for D and D^2 can be found in the literature [28]. Notice that D^2 and D^4, the second- and fourth-order spectral differentiation matrices respectively, are centrosymmetric as long as the collocation points are symmetric about zero, as is the case for Chebyshev and Legendre points.

Let $A \otimes B$ denote the Kronecker product of matrices A and B.

Proposition 1 *If $A \in \mathbb{R}^{n\times n}$ and $B \in \mathbb{R}^{m\times m}$ are centrosymmetric, then $A \otimes B$ is centrosymmetric.*

Proof Let J_n denote the flip matrix of size n. Then

$$(J_n \otimes J_m)(A \otimes B)(J_n \otimes J_m) = (J_n A J_n \otimes J_m B J_m) = A \otimes B.$$

Therefore, $A \otimes B$ is centrosymmetric.

We consider the following PDEs and the associated centrosymmetric linear systems arising from applying spectral discretization:

- *2D Poisson equation (sparse):* Consider the Poisson equation with homogeneous Dirichlet boundary conditions in the square domain $(-1, 1)^2$. The second-order spectral differentiation matrix is

$$\hat{\mathcal{A}}_{2DP} = -([[D^2]] \otimes I_{N-1}) - (I_{N-1} \otimes [[D^2]]). \tag{5}$$

  Here, I_{N-1} denotes the identity matrix of size $N-1$ and $[[D^2]]$ is a matrix that is obtained from D^2 by removing the first and last rows and columns. The condition number of this matrix is $O(N^4)$; see [31].
- *2D biharmonic equation (sparse+dense):* Consider the biharmonic equation with homogeneous Dirichlet boundary conditions in the square domain $(-1, 1)^2$. The fourth-order spectral differentiation matrix is

$$\hat{\mathcal{A}}_{2DB} = (B \otimes I_{N-1}) + (I_{N-1} \otimes B) + 2([[D^2]] \otimes [[D^2]]), \tag{6}$$

  where B is a spectral approximation of the fourth derivative, taking into account the boundary conditions. Consider $Y(x) = (1 - x^2)Z(x)$, with $Z(\pm 1) = 0$. Then, $Y(\pm 1) = Y'(\pm 1) = 0$ and $Y''''(x) = (1 - x^2)Z''''(x) - 8xZ'''(x) - 12Z''(x)$. Therefore, a spectral approximation of the fourth derivative, imposing the boundary conditions, is given by

$$B = (M\,[[D^4]] - 8V[[D^3]] - 12[[D^2]])\, M^{-1},$$

  where M and V are $(N-1)\times(N-1)$ diagonal matrices with diagonal entries $1-x_i^2$ and x_i, respectively. This matrix is extremely ill-conditioned, the condition number is $O(N^8)$. See [32]. Since the matrix consists of a summation of two matrices, a sparse matrix $(B \otimes I_{N-1}) + (I_{N-1} \otimes B)$, and a dense matrix $2([[D^2]] \otimes [[D^2]])$, we refer to it as "sparse+dense."

- *3D Poisson equation (sparse):* Consider the Poisson equation with homogeneous boundary conditions in the cubic domain $(-1, 1)^3$. The 3D second-order spectral differentiation matrix is

$$\hat{\mathcal{A}}_{3DP} = -([[D^2]] \otimes I_{N-1} \otimes I_{N-1}) - (I_{N-1} \otimes [[D^2]] \otimes I_{N-1}) \\ + (I_{N-1} \otimes I_{N-1} \otimes [[D^2]]). \tag{7}$$

- *3D Helmholtz equation (sparse):* Consider the indefinite Helmholtz equation

$$-(\Delta + k^2)u = f, \qquad \text{in } (-1, 1)^3, \tag{8}$$

where k is a constant called wave number. We assume homogeneous Dirichlet boundary conditions. The spectral discretization of this equation gives

$$\hat{\mathcal{A}}_{3DH} = \hat{\mathcal{A}}_{3DP} - k^2 I_{(N-1)^3}. \tag{9}$$

- *2D diffusion equation (sparse):* Consider the anisotropic diffusion equation

$$-\nabla \cdot (a(x, y)\nabla u) = f(x, y), \qquad \text{in } (-1, 1)^2, \tag{10}$$

with homogeneous Dirichlet boundary conditions and $a(x, y) \in C^\infty$ such that $0 < k_1 \leq a(x, y) \leq k_2$. Ignoring the boundary conditions, the spectral matrix for this operator is

$$\mathcal{A}_{2DPV} = -(D \otimes I_{N+1})S(D \otimes I_{N+1}) - (I_{N+1} \otimes D)S(I_{N+1} \otimes D), \tag{11}$$

where S is a diagonal matrix

$$S = \text{diag}(\text{vec}(Z)), \tag{12}$$

with $Z_{ij} = a(x_i, y_j),\ 0 \leq i, j \leq N$, x_i and y_j are the Chebyshev Gauss Lobatto points; $\text{vec}(Z)$ is the vector representation of Z. For $\mathcal{A}_{2DPV}$ to be centrosymmetric, the diagonal matrix S must be centrosymmetric. Notice that the Chebyshev (Legendre) collocation points are symmetric about the origin. Assuming $a(x, y)$ is even in x and in y, then

$$\begin{aligned} &a(x_0, y_0) = a(x_N, y_N), \quad a(x_1, y_0) = a(x_{N-1}, y_N), \ldots, a(x_N, y_0) = a(x_0, y_N), \\ &a(x_0, y_1) = a(x_N, y_{N-1}), \ a(x_1, y_1) = a(x_{N-1}, y_{N-1}), \ldots, a(x_N, y_1) = a(x_0, y_{N-1}), \\ &\vdots \\ &a(x_0, y_N) = a(x_N, y_0), \quad a(x_1, y_N) = a(x_{N-1}, y_0), \ldots, a(x_N, y_N) = a(x_0, y_0), \end{aligned}$$

and therefore, S is centrosymmetric. To implement the boundary conditions, we remove appropriate rows and columns from the matrix. The new matrix, which we denote by $\hat{\mathcal{A}}_{2DPV}$, is still centrosymmetric.

- *2D variable-coefficient biharmonic equation (sparse+dense)*:

$$\begin{aligned}\Delta(a(x,y)\,\Delta u) = f(x,y) \qquad & \text{in } \Omega = (-1,1)^2 \\ u = 0 \qquad & \text{on } \partial\Omega \\ \frac{\partial u}{\partial \nu} = 0 \qquad & \text{on } \partial\Omega,\end{aligned} \tag{13}$$

where $a(x,y) \in C^{\infty}(\Omega)$ such that $0 < k_1 \leq a(x,y) \leq k_2$. It is not straightforward to apply the spectral collocation method to the biharmonic operator with variable coefficient, especially imposing the boundary conditions. Without considering the boundary conditions, the spectral differentiation matrix for this operator is

$$\begin{aligned}\mathcal{A}_{2DBV} = & (D^2 \otimes I_{N+1})S(E \otimes I_{N+1}) + (I_{N+1} \otimes D^2)S(I_{N+1} \otimes E) \\ & + (D^2 \otimes I_{N+1})S(I_{N+1} \otimes E) + (I_{N+1} \otimes D^2)S(E \otimes I_{N+1}),\end{aligned} \tag{14}$$

where S is given by (12) and E is a spectral approximation of the second derivative, taking into account both boundary conditions. Same as for the diffusion equation, we assume $a(x,y)$ is even in x and in y, so that S is centrosymmetric. Notice that usually, the second-order derivative needs just boundary conditions $u(\pm 1) = 0$. Let $Y(x) = (1-x^2)Z(x)$, with $Z(\pm 1) = 0$. Therefore, $Y(\pm 1) = Y'(\pm 1) = 0$ and $Y'' = (1-x^2)Z''-4xZ'-2Z$, leading to $E = (MD^2-4VD-2I)\,M^{-1}$ as a spectral approximation of the second derivative imposing both boundary conditions, where M and V are diagonal matrices with diagonal entries $1-x_i^2$ and x_i, respectively. Notice that in (14), we have two different types of spectral second-derivative matrices, D^2 and E. The reason is that the solution satisfies both boundary conditions, but Δu does not satisfy any boundary condition. Finally, to implement the boundary condition $u = 0$ (corresponding to $Z(\pm 1) = 0$), we remove the appropriate rows and columns of the matrix (14). The resulting matrix, which we denote by $\hat{\mathcal{A}}_{2DBV}$, is centrosymmetric but dense. This matrix has a structure similar to the discrete 2D biharmonic case; it consists of a summation of a sparse matrix and a dense one; therefore, we call it sparse+dense.

- *Poisson equation with Dirichlet boundary conditions (sparse, SPD)*: Consider the one-dimensional problem $-u'' = f(x)$ with homogeneous boundary conditions, $u(\pm 1) = 0$. Multiplying both sides by the Lagrange polynomial ℓ_j for $1 \leq j \leq N-1$ and integrating by parts, we obtain

$$\int_{-1}^{1} u'\ell_j' = \int_{-1}^{1} f\ell_j.$$

Using a quadrature formula involving Legendre collocation points, an approximation of this equation is

$$\sum_{k=0}^{N} u'(x_k)\ell_j'(x_k)\rho_k = \sum_{k=0}^{N} f(x_k)\ell_j(x_k)\rho_k, \qquad 0 \leq 1 \leq N-1.$$

This is equivalent to

$$\sum_{k=0}^{N}(Du_h)_k D_{kj}\rho_k = f(x_j)\rho_j, \qquad 1 \le j \le N-1,$$

where u_h is the vector containing the approximate solution at collocation points. Since the solution vanishes at the end points, we redefine u_h by removing its first and last components. Then, the matrix form of above equation is

$$[[D^T WD]]\, u_h = [[W]] f_h,$$

where W is a diagonal matrix with diagonal entries ρ_j and f_h is f evaluated at the interior collocation points. Define $\mathcal{C} = [[D^T WD]]$, then the above calculation shows $-[[D^2]] = \mathcal{C}\,[[W]]^{-1}$. The matrix $\mathcal{C}$ is symmetric positive semidefinite and its condition number is $O(N^3)$ [31].
The Legendre spectral method for the PDE

$$\begin{aligned} -\Delta u &= f(x, y) \qquad \text{in } \Omega = (-1, 1)^2 \\ u &= 0 \qquad\qquad\quad \text{on } \partial\Omega, \end{aligned} \tag{15}$$

leads to

$$\big(-(I_{N-1} \otimes [[D^2]]) - ([[D^2]] \otimes I_{N-1})\big)u_h = f_h.$$

Let $\hat{W} := [[W]]$. Multiplying the above equation by $\hat{W}^{-1/2} \otimes \hat{W}^{-1/2}$, we obtain

$$\big((I_{N-1} \otimes M) + (M \otimes I_{N-1})\big)\, v_h = (\hat{W}^{1/2} \otimes \hat{W}^{1/2}) f_h, \tag{16}$$

where $M = \hat{W}^{-1/2}\mathcal{C}\hat{W}^{-1/2}$ and $v_h = (\hat{W}^{1/2} \otimes \hat{W}^{1/2})u_h$. Observe that M is SPD, since $\mathcal{C}$ is SPD and by Sylvester's theorem for congruent transformation, the number of positive eigenvalues of M is the same as the number of positive eigenvalues of $\mathcal{C}$. Therefore,

$$\mathcal{A}_{2DPS} = (I_{N-1} \otimes M) + (M \otimes I_{N-1}), \tag{17}$$

is SPD, centrosymmetric and sparse.

- *Neumann problem (sparse, SPD)*: We first consider the 1D Neumann problem

$$-u'' + u = f(x), \qquad u'(-1) = u'(1) = 0.$$

Multiply the ODE by the Lagrange polynomial ℓ_j for $0 \le j \le N$ and integrate by parts to obtain

$$\int_{-1}^{1}(u'\ell_j' + u\ell_j) = \int_{-1}^{1} f\ell_j,$$

apply a quadrature formula involving Legendre collocation points, to obtain an approximation of this equation

$$\sum_{k=0}^{N}\big(u'(x_k)\ell'_j(x_k)+u(x_k)\ell_j(x_k)\big)\rho_k=\sum_{k=0}^{N}f(x_k)\ell_j(x_k)\rho_k,\qquad 0\le j\le N.$$

This is equivalent to

$$\sum_{k=0}^{N}(Du_h)_k D_{kj}\rho_k+(u_h)_j\rho_j=f(x_j)\rho_j,\qquad 0\le j\le N,$$

where u_h is the vector containing the approximates solution at collocation points. The matrix form of the above equation is $(D^T WD+W)u_h=Wf_h$. Therefore, a symmetric Legendre spectral method for the 2D Neumann problem

$$\begin{aligned} -\Delta u+u=f(x,y) &\qquad \text{in } \Omega=(-1,1)^2\\ \frac{\partial u}{\partial \nu}=0 &\qquad \text{on } \partial\Omega, \end{aligned} \tag{18}$$

leads to the discrete problem [31]

$$\big((B\otimes W)+(W\otimes B)+(W\otimes W)\big)u_h=(W\otimes W)f_h, \tag{19}$$

where $B=D^T WD$. Notice that

$$\mathcal{A}_{2DPN}=(B\otimes W)+(W\otimes B)+(W\otimes W), \tag{20}$$

is SPD, centrosymmetric and sparse.

- *Poisson equation with Robin boundary conditions (sparse, SPD, nearly centrosymmetric)*: We apply the Legendre-Galerkin method to the problem

$$\begin{aligned} -\Delta u=f(x,y) &\qquad \text{in } \Omega=(-1,1)^2\\ \frac{\partial u}{\partial \nu}+a(x,y)u=0 &\qquad \text{on } \partial\Omega, \end{aligned} \tag{21}$$

where $a(x,y)\ge k>0$ and $a(x,y)$ is bounded and sufficiently smooth. The weak form of this PDE is

$$\int_{\partial\Omega} auv+\int_{\Omega}\nabla u\cdot\nabla v=\int_{\Omega} fv,\qquad \forall v\in H^1(\Omega).$$

The associated bilinear form is coercive. Replacing $v=\ell_p(x)\ell_q(y)$ for $0\le p,q\le N$ and using a quadrature formula with Legendre collocation points, we obtain the system $\mathcal{A}_{2DPR}\,u_h=(W\otimes W)f_h$, where

$$\mathcal{A}_{2DPR}=C+(B\otimes W)+(W\otimes B), \tag{22}$$

where $B = D^T W D$, and the matrix C is the diagonal matrix

$$C = \mathrm{diag}(\mathrm{vec}(Z)\,), \tag{23}$$

and Z is an $(N+1) \times (N+1)$ matrix

$$\begin{bmatrix} a(x_0, y_0) & a(x_1, y_0) & \ldots & a(x_{N-1}, y_0) & a(x_N, y_0) \\ a(x_0, y_1) & 0 & \ldots & 0 & a(x_N, y_1) \\ \vdots & \vdots & & \vdots & \vdots \\ a(x_0, y_{N-1}) & 0 & \ldots & 0 & a(x_N, y_{N-1}) \\ a(x_0, y_N) & a(x_1, y_N) & \ldots & a(x_{N-1}, y_N) & a(x_N, y_N) \end{bmatrix}.$$

The matrix $\mathcal{A}_{2DPR}$ is sparse but not centrosymmetric unless a is even in x and y. It is nearly centrosymmetric in the sense that it is centrosymmetric except along the diagonal.

- *Helmholtz equation with Robin boundary conditions (sparse, nearly centrosymmetric)*: We consider the 2D Helmholtz equation with Robin boundary conditions

$$\begin{aligned} -(\Delta + k^2)u &= f(x, y) \qquad \text{in } \Omega = (-1, 1)^2 \\ \frac{\partial u}{\partial \nu} + a(x, y)u &= 0 \qquad \text{on } \partial\Omega, \end{aligned} \tag{24}$$

where k is a positive constant. Using the weak form of this PDE, the spectral discretization of this equation is given by

$$\mathcal{A}_{2DHR} = C + (B \otimes W) + (W \otimes B) - k^2(W \otimes W), \tag{25}$$

where $B = D^T W D$ and C is defined by (23). This matrix is sparse, symmetric and nearly centrosymmetric.

3 An incomplete double-cone factorization

In the sequel, we use standard notation for floor $\lfloor a \rfloor$ and ceiling $\lceil a \rceil$ of a real number a. The remainder of an integer n divided by an integer k is denoted by $(n \bmod k)$.

Definition 1 Let $n \geq 3$. For a given k, $1 \leq k \leq \lceil n/2 \rceil - 1$, consider the following two-column sub-matrix of $A = (a_{ij}) \in \mathbb{R}^{n \times n}$,

$$\begin{bmatrix} a_{k+1,k} & a_{k+1,n-k+1} \\ \vdots & \vdots \\ a_{n-k,k} & a_{n-k,n-k+1} \end{bmatrix}.$$

The matrix A is called a vertical double-cone, or v-double-cone, if every two-column sub-matrix of A has all zero entries for each $1 \leq k \leq \lceil n/2 \rceil - 1$.

Definition 2 Let $n \geq 3$. For a given $k,\ 1 \leq k \leq \lceil n/2 \rceil - 1$, consider the following two-row sub-matrix of $A = (a_{ij}) \in \mathbb{R}^{n \times n}$,

$$\begin{bmatrix} a_{k,k+1} & \cdots & a_{k,n-k} \\ a_{n-k+1,k+1} & \cdots & a_{n-k+1,n-k} \end{bmatrix}.$$

The matrix A is called a horizontal double-cone, or h-double-cone, if every two-row sub-matrix of A has all zero entries for each $1 \leq k \leq p$, where $p = \lceil n/2 \rceil - 1$.

We call a matrix "*double-cone*" if it is either v-double-cone or h-double-cone. This definition extends the one given by Burnik [24] to horizontal double-cone matrices.

Example 1 Examples of matrices that have a double-cone nonzero structure are

$$A_1 = \begin{bmatrix} * & * & * & * & * \\ & * & * & * & \\ & & * & & \\ & * & * & * & \\ * & * & * & * & * \end{bmatrix}, \qquad A_2 = \begin{bmatrix} * & * & * & * \\ & * & * & \\ & * & * & \\ * & * & * & * \end{bmatrix}, \qquad A_3 = \begin{bmatrix} * & & & & & * \\ * & * & & & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & & & * & * \\ * & & & & & * \end{bmatrix},$$

where A_1 and A_2 are v-double-cone and A_3 is h-double-cone.

For a nonsingular matrix A, the LU factorization generates a unit lower triangular matrix L, an invertible upper triangular matrix U, and a permutation matrix P such that $PA = LU$. Solving a linear system $Ax = b$ via the LU factorization costs $\frac{2}{3}n^3 - n^2 + O(n)$, where n is the dimension of the matrix [33, 34].

In the following, we show how to construct double-cone factorization for centrosymmetric matrices. For a nonsingular $\mathcal{A} \in \mathcal{C}_n$ with n even, each diagonal block in the similarity transformation (2) of $\mathcal{A}$ is nonsingular. Then, there are unit lower triangular matrices L_1 and L_2 and nonsingular upper triangular matrices U_1 and U_2 such that

$$P_1(A + JC) = L_1U_1, \qquad P_2(A - JC) = L_2U_2,$$

where P_1 and P_2 are permutation matrices. Thus,

$$\begin{aligned} \mathcal{A} &= \mathcal{U} \begin{bmatrix} A + JC & 0 \\ 0 & A - JC \end{bmatrix} \mathcal{U}^T = \mathcal{U} \begin{bmatrix} P_1^T L_1 U_1 & 0 \\ 0 & P_2^T L_2 U_2 \end{bmatrix} \mathcal{U}^T \\ &= \mathcal{U} \begin{bmatrix} P_1^T & 0 \\ 0 & P_2^T \end{bmatrix} \mathcal{U}^T \mathcal{U} \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} \mathcal{U}^T \mathcal{U} \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \mathcal{U}^T = Q^T X Y, \end{aligned}$$

where

$$Q = \mathcal{U} \begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix} \mathcal{U}^T = \frac{1}{2} \begin{bmatrix} P_1 + P_2 & (P_1 - P_2)J \\ J(P_1 - P_2) & J(P_1 + P_2)J \end{bmatrix}, \tag{26}$$

is an orthogonal centrosymmetric matrix since the permutation matrices P_1 and P_2 are orthogonal. The matrix X is defined as

$$X = \mathcal{U} \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} \mathcal{U}^T = \frac{1}{2} \begin{bmatrix} L_1 + L_2 & (L_1 - L_2)J \\ J(L_1 - L_2) & J(L_1 + L_2)J \end{bmatrix}. \tag{27}$$

It is centrosymmetric h-double-cone since L_1 and L_2 are lower triangular matrices. The matrix Y is given by

$$Y = \mathcal{U} \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \mathcal{U}^T = \frac{1}{2} \begin{bmatrix} U_1 + U_2 & (U_1 - U_2)J \\ J(U_1 - U_2) & J(U_1 + U_2)J \end{bmatrix}, \tag{28}$$

and it is centrosymmetric v-double-cone. If n is odd, then the notation is a bit more cumbersome, but the same process can be followed.

We conclude that for a centrosymmetric matrix $\mathcal{A} \in \mathcal{C}_n$, applying the LU factorization to each diagonal block of (2) leads to a factorization of the form

$$Q\mathcal{A} = XY,$$

where Q is centrosymmetric orthogonal, and X and Y are centrosymmetric double-cones. We call this the *double-cone factorization, or XY factorization*, of a centrosymmetric matrix. Since $\mathcal{A}$ is nonsingular, both X and Y are nonsingular. Therefore, the solution of the linear system $\mathcal{A}z = b$ can be computed by solving $Xw = \hat{b}$, where $\hat{b} = Qb$, followed by $Yz = w$. These linear systems involve double-cone matrices and can be solved by using a modified backward substitution [24].

The double-cone factorization to solve a centrosymmetric system requires $\frac{1}{6}n^3 + O(n^2)$ flops, which is asymptotically four times faster than solving by a standard LU factorization. This is the same speed up as the approach suggested by Andrew in [16].

Example 2 We consider the matrix from the Chebyshev collocation discretization of the 1D Helmholtz equation $-u'' - 10u = f$ with homogeneous Dirichlet boundary conditions and with six Chebyshev Gauss Lobatto points. Then,

$$\mathcal{A} = \begin{bmatrix} 52.66 & -24.39 & 6.66 & -3.60 & 2.66 \\ -13.10 & 7.33 & -9.33 & 2.66 & -1.55 \\ 2.66 & -8.00 & 2.66 & -8.00 & 2.66 \\ -1.55 & 2.66 & -9.33 & 7.33 & -13.10 \\ 2.66 & -3.60 & 6.66 & -24.39 & 52.66 \end{bmatrix},$$

and the XY factorization is given by $Q\mathcal{A} = XY$, where

$$Q = \begin{bmatrix} 1.00 & 0 & 0 & 0 & 0 \\ 0 & 0.50 & 0.70 & -0.50 & 0 \\ 0 & 0.70 & 0 & 0.70 & 0 \\ 0 & -0.5 & 0.70 & 0.50 & 0 \\ 0 & 0 & 0 & 0 & 1.00 \end{bmatrix},$$

and

$$X = \begin{bmatrix} 1.00 & 0 & 0 & 0 & 0 \\ -0.08 & 1.00 & 0 & 0 & 0.14 \\ -0.18 & -0.19 & 1.00 & -0.19 & -0.18 \\ 0.14 & 0 & 0 & 1.00 & -0.08 \\ 0 & 0 & 0 & 0 & 1.00 \end{bmatrix}, \quad Y = \begin{bmatrix} 52.66 & -24.39 & 6.66 & -3.60 & 2.66 \\ 0 & -4.76 & 1.43 & -4.63 & 0 \\ 0 & 0 & -10.14 & 0 & 0 \\ 0 & -4.63 & 1.43 & -4.76 & 0 \\ 2.66 & -3.60 & 6.66 & -24.39 & 52.66 \end{bmatrix}.$$

It is straightforward to adapt the proposed factorization to centrosymmetric symmetric positive definite matrices. Notice that the number of flops for solving such an SPD system using the Cholesky factorization is half of the flop count using LU factorization, that is, $\frac{1}{3}n^3 + O(n^2)$, where n is the size of the matrix [35]. Here, we will develop a special form of double-cone factorization to solve a centrosymmetric SPD linear system. The algorithm is same as general centroisymmetric matrices, except we replace the LU factorization for each diagonal block in the similarity transformation of the matrix by a Cholesky factorization. The result is a factorization of the form XX^T, where X is a centrosymmetric double-cone. We call it the XX^T factorization.

Let $\mathcal{A} \in \mathcal{C}_n$ be SPD with n even. Consider the similarity transformation of $\mathcal{A}$ given by (2). Recall that if $\mathcal{A}$ is SPD, then the diagonal blocks $A \pm JC$ are SPD. Then, there are lower triangular matrices L_1 and L_2 with positive diagonal entries such that $A + JC = L_1 L_1^T$ and $A - JC = L_2 L_2^T$, (pivoting is not necessary for Cholesky factorization). Therefore,

$$\begin{aligned} \mathcal{A} &= \mathcal{U} \begin{bmatrix} A + JC & 0 \\ 0 & A - JC \end{bmatrix} \mathcal{U}^T = \mathcal{U} \begin{bmatrix} L_1 L_1^T & 0 \\ 0 & L_2 L_2^T \end{bmatrix} \mathcal{U}^T \\ &= \mathcal{U} \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} \mathcal{U}^T \mathcal{U} \begin{bmatrix} L_1^T & 0 \\ 0 & L_2^T \end{bmatrix} \mathcal{U}^T = X\,X^T, \end{aligned}$$

where X is a centrosymmetric h-double-cone matrix

$$X = \mathcal{U} \begin{bmatrix} L_1 & 0 \\ 0 & L_2 \end{bmatrix} \mathcal{U}^T = \frac{1}{2} \begin{bmatrix} L_1 + L_2 & (L_1 - L_2)J \\ J(L_1 - L_2) & J(L_1 + L_2)J \end{bmatrix}. \tag{29}$$

The case where the size of the matrix n is odd follows almost exactly the same steps, with small modifications. It can be checked that solving an SPD centrosymmetric system by using double-cone XX^T factorization takes $\frac{1}{12}n^3 + O(n^2)$ flops.

Iterative methods such as Krylov subspace methods, combined with effective preconditioners, are efficient for systems of linear equations involving large sparse matrices. Different preconditioners have been proposed for spectral differentiation matrices in the literature. These include preconditioners based on finite difference approximations [36–38], finite-element methods [39, 40], integration preconditioners [41, 42], and Kronecker product approximation preconditioners [43, 44]. Most of these preconditioners were tested on 1D and 2D Poisson equations, and some were applied to the Helmholtz equation and other PDEs. The effectiveness of incomplete LU factorizations [45, 46] as preconditioners is illustrated in Canuto et al. [27] for a finite-difference discretization based on a Chebyshev collocation nodes to the 2D Poisson equation.

There are relatively few papers on efficient preconditioners for the system arising from the biharmonic equation with homogeneous Dirichlet boundary conditions in square domains using spectral methods. This corresponding matrix is extremely ill-conditioned. Funaro and Heinrichs [47] analyzed the Legendre and Chebyshev spectral collocation for the 1D fourth-order biharmonic equation and proposed a finite-difference preconditioner for the system based at collocation nodes. They also introduced a preconditioner by squaring the second-order centered finite-difference matrix of the Laplacian. Heinrichs [48] solved the 2D problem by splitting it into a system of two equations with the Laplace operator. The new system is solved by a Chebyshev collocation method preconditioned by a finite-difference scheme.

Incomplete LU factorizations (ILU) [46] are widely used as preconditioners for large and sparse systems. They come in a few distinct types. We consider (i) ILU(0), which is based on prescribing the sparsity pattern of the factors ahead of time, and (ii) ILUTP, where the nonzero pattern is determined dynamically throughout the computation by discarding elements that are below a certain prescribed drop tolerance.

The standard ILU factorization, being intended for general matrices, does not take advantage of centrosymmetry. In deriving a new structure-preserving preconditioner, we compute the IXY(0) factorization or the IXYTP factorization of a centrosymmetric $\mathcal{A}$ from the ILU(0) factorizations or the ILUTP factorizations, respectively, of the two diagonal blocks in the similarity transformation (2). We expect savings in memory requirements and computational work, since the computed factors are of blocks that are half the size of the original matrix, resulting in a reduction in execution time. In Fig. 1, the sparsity pattern of the 3D second-order spectral differentiation matrix and its IXY(0) factorization are given. Notice that we only need to store one-half of those entries due to centrosymmetry. We can see in Fig. 1 that X and Y have a sparsity pattern that is different from that of the original matrix. This is due to the way in which we compute X and Y in (27) and (28). The factors have the sparsity patterns of the diagonal blocks, but we add or subtract them from each other, and therefore, some extra nonzero elements are generated.

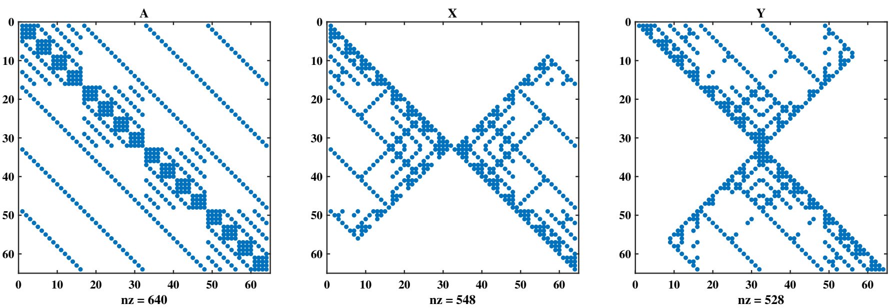

Fig. 1 Sparsity pattern of 3D second-order Chebyshev spectral differentiation matrix and its IXY(0) factorization

For sparse centrosymmetric SPD matrices, we develop an incomplete double-cone factorization that we call IXX in a manner similar to the IXY factorization: we compute the incomplete Cholesky factorization (ICHOL) of the two diagonal blocks of (2). Here, too, we consider two types: IXX(0) and IXXT. To take advantage of the centrosymmetric structure of the matrices, we implement the Melman [29] and Fassbender and Ikramov [30] methods for fast matrix–vector products, which speed up the calculations in PCG and GMRES. We also use the modified backward substituation proposed in [24] to solve double-cone centrosymmetric linear systems inside the iterative solvers.

4 Numerical results

In this section, we demonstrate the performance of the new incomplete factorizations as preconditioners for Krylov subspace solvers. Our Krylov subspace solvers are GMRES in the general nonsymmetric case and PCG in the SPD case. We conducted numerical experiments using a Dell laptop with a 1.9 GHz Intel Core i7 CPU.

Details of parameters of PDEs used for numerical experiments are given in Table 1. For the 2D diffusion equation and variable-coefficient biharmonic equation, we consider the PDEs in two cases,

$$a_1(x, y) = 1 + kx^2y^2, \qquad \text{or} \qquad a_2(x, y) = 1 + kx^2y^4, \tag{30}$$

where k is positive constant. Both functions are even in x and in y. The first one is symmetric, ($a_1(x, y) = a_1(y, x)$), while the second one is not. For the 2D Poisson equation with homogeneous Robin boundary conditions, we consider $a(x, y) = 2+x$. The corresponding matrices are either centrosymmetric or nearly centrosymmetric; some are dense, while others are sparse.

Table 1 List of PDEs used for numerical experiments

Name	PDE	Exact solution	Sparsity
1DP	1D Poisson equation	$\sin(\pi x)$	Dense
2DP	2D Poisson equation	$\sin(\pi x)\sin(\pi y)$	Sparse
3DP	3D Poisson equation	$\sin(\pi x)\sin(\pi y)\sin(\pi z)$	Sparse
2DPV	2D diffusion equation	$\sin(\pi x)\sin(\pi y)$	Sparse
2DPS	2D Poisson equation	$\sin(\pi x)\sin(\pi y)$	SPD sparse
2DPN	2D Neumann problem	$(1-x^2)^2\cos(\pi y)$	SPD sparse
2DPR	2D Poisson equation with Robin BC	$e^y(1-x^2)^2(1-y^2)^2$	Sparse
1DB	1D biharmonic equation	$1+\cos(\pi x)$	Dense
2DB	2D biharmonic equation	$(1+\cos(\pi x))(1-y^2)^2$	Sparse+dense
2DBV	2D biharmonic with variable coefficient	$\sin^2(\pi x)\sin^2(\pi y)$	Sparse+dense
3DH	3D Helmholtz equation	$\sin(\pi x)\sin(\pi y)\sin(\pi z)$	Sparse

Example (i). The 2D and 3D Poisson and diffusion equations We solve the 2D and 3D Poisson and 2D diffusion problems and examine the performance of the incomplete factorization preconditioners. For this example, we also define a cross-Jacobi preconditioner, which consists of the diagonal and anti-diagonal entries of $\mathcal{A}$ and preserves centrosymmetry. We compare it against a standard Jacobi preconditioner.

Figure 2 shows the convergence of GMRES for the linear systems with the 2D and 3D second-order Chebyshev differentiation matrices; the dimensions of the matrices are 400×400 and 8000×8000, respectively. For ILUTP and IXYTP, a drop tolerance of 10^{-3} is used, and the iteration counts are significantly lower than for ILU(0) and IXY(0), respectively. GMRES needs 134 iteration to converge in the 2D case, while with the IXYTP or ILUTP factors as preconditioners GMRES converges in fewer than four iterations. For the 3D case, GMRES needs 213 iteration to converge, while with the IXYTP or ILUTP factors as preconditioners, it converges in six iterations. The cross-Jacobi and Jacobi preconditioners perform identically to each other but require many more iterations compared to the incomplete factorization and are not competitive.

In Table 2, we compare the convergence of GMRES for solving the 2D and 3D Poisson equations with preconditioners given by the ILU(0), IXY(0), ILUTP, and IXYTP factorizations, with different values of "tol," the drop tolerance used in ILUTP and IXYTP. The density factor is defined as

$$d_{LU} = \frac{nnz(L) + nnz(U) - n}{nnz(A)}, \tag{31}$$

for an LU factorization, where $nnz(L)$ denotes the number of non-zero elements in a given matrix L and n is the size of the matrix. The density factor for other factorizations is defined in a similar manner. For ILUTP and IXYTP, we need to choose a drop tolerance judiciously to avoid having a nearly or completely filled-in factorization approaching the density of LU or XY. The table shows that the drop tolerance 10^{-3} gives the best results.

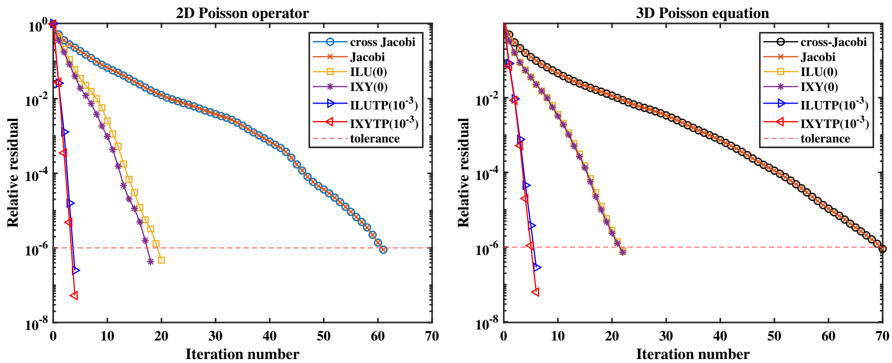

Fig. 2 Convergence of GMRES with the proposed preconditioner for 2D (left) and 3D (right) second-order Chebyshev spectral differentiation matrices

Table 2 Results of applying the ILU(0), IXY(0), ILUTP, and IXYTP factorizations (with different drop tolerances) as preconditioners for GMRES. The definition of the parameter $d_{ixy(0)}$ is given in (31) and the text that follows, notice that $d_{ilu(0)} = 1$. The parameter $N_{ilu(0)}$ denotes the number of iterations in GMRES preconditioned by ILU(0); $N_{ixy(0)}$, N_{ilutp}, and N_{ixytp} are similarity defined for IXY(0), ILUTP, and IXYTP respectively

$\mathcal{A}$	$\mathbf{d_{lu}}$	$\mathbf{d_{ixy(0)}}$	$\mathbf{N_{ilu(0)}}$	$\mathbf{N_{ixy(0)}}$	**tol**	$\mathbf{d_{ilutp}}$	$\mathbf{d_{ixytp}}$	$\mathbf{N_{ilutp}}$	$\mathbf{N_{ixytp}}$
					10^{-2}	0.61	0.88	8	7
2DP	9.79	1.85	19	17	10^{-3}	1.72	2.64	4	4
					10^{-4}	3.45	5.13	3	2
					10^{-2}	1.10	1.86	9	8
2DPV	9.79	1.85	19	16	10^{-3}	2.89	4.84	4	4
$a = 1 + 10x^2y^2$					10^{-4}	5.75	7.66	3	3
					10^{-2}	0.47	0.66	10	10
3DP	131.38	1.88	22	21	10^{-3}	1.86	3.05	6	6
					10^{-4}	6.06	9.81	4	4

Figure 3 shows the convergence of GMRES with the IXY(0) and IXYTP preconditioners for the Chebyshev differentiation matrix arising from solving the diffusion equation (10) for $a(x, y) = 1 + 10x^2y^2$. The results are compared with ILU(0), ILUTP, cross-Jacobi, and Jacobi preconditioners. For the corresponding linear system of dimensions 400×400, GMRES without a preconditioner needs approximately 209 iterations to achieve the desired reduction in relative residual norm. The IXYTP factorization preconditioner with drop tolerance 10^{-3} has a density factor of 4.84, and it converges in four iterations, while IXY(0) has a density factor of 1.85, and it

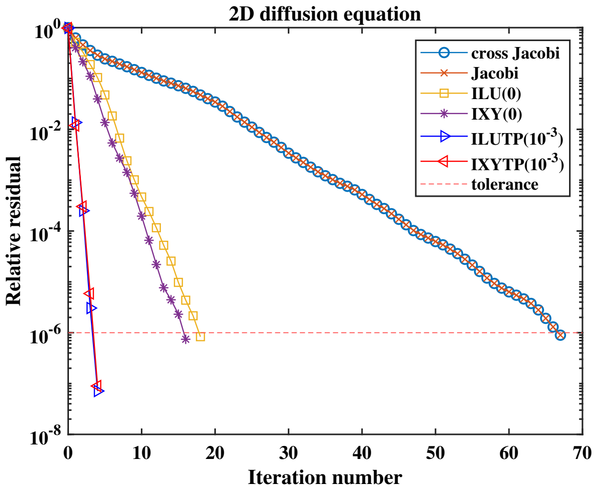

Fig. 3 Convergence of GMRES with the proposed preconditioners for the 2D diffusion equation

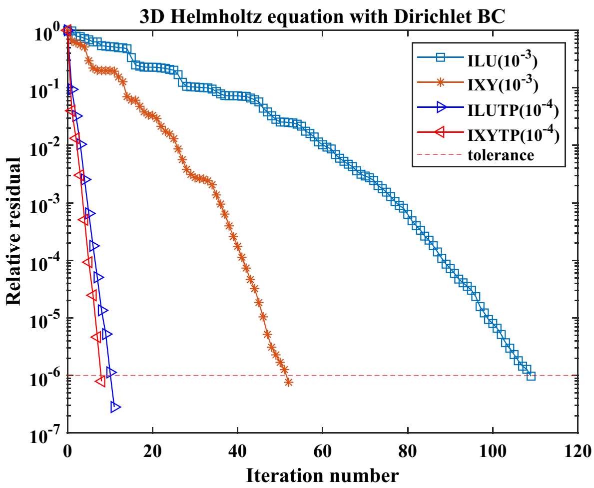

Fig. 4 Convergence of GMRES for the 3D Helmholtz equation

converges in 16 iterations to the same reduction in relative residual norm. The Jacobi and the cross-Jacobi preconditioners are, again, not at all competitive, and we do not pursue them further in the examples that follow.

Example (ii). 3D Helmholtz equation We consider the Helmholtz equation (8) with homogeneous boundary conditions in a 3D cubic domain with different wave numbers. We fix $N = 20$, resulting in an indefinite matrix of size 8000×8000. We use Chebyshev collocation to obtain the linear system (9) associated with this PDE. The convergence results for GMRES with IXYTP and ILUTP factors as preconditioners with drop tolerance 10^{-3} and 10^{-4} are compared in Fig. 4. For this example, $k^2 = 1200$ and the condition number of the associated linear system are 5.06×10^4.

Table 3 shows the number of iterations needed for GMRES with the ILUTP and IXYTP factorizations as preconditioners. We experiment with a few linear systems of size 8000×8000 corresponding to different wave numbers, k. To test the robustness of our solution approach, we aim to solve difficult instances of the problem: we select values of k^2 close to eigenvalues of the 3D discrete Laplacian spectral operator; the coefficient matrices tested have a relatively large condition number. For this challenging problem, the results are mixed. For small wave numbers, IXY(0) and ILU(0)

Table 3 Condition numbers and iteration counts for ILUTP(10^{-4}) and IXYTP(10^{-4}) factors applied as preconditioners for iteratively solving the 3D Helmholtz using different wave numbers. Condition numbers are very sensitive to k; hence, we show 4 digits after the decimal point to achieve a large condition number

k^2	$\kappa(\mathcal{A})$	$\mathbf{N}_{\mathbf{ilutp}(10^{-4})}$	$\mathbf{N}_{\mathbf{ixytp}(10^{-4})}$
219.5988	3.68×10^9	62	53
2195.9064	1.65×10^{11}	53	41
3362.1876	3.13×10^8	31	24

perform well, but they mostly fail to converge as the wave numbers become larger, so we deem them less reliable and do not present their results. The performance of ILUTP and IXYTP with drop tolerance 10^{-4} is consistent, and convergence requires 18–62 iterations. We use full GMRES to highlight the effectiveness of preconditioning; since the matrices are not large, this can be done without paying a prohibitive computational cost or allocating a prohibitive amount of storage. We note that restarted GMRES(ℓ) with various values of ℓ often led to large iteration numbers for all preconditioners for several values of k that have been tested.We suspect this is due to the density of eigenvalues of the preconditioned matrix near 0. Without preconditioners (full), GMRES does not converge even within several hundreds of iterations.

The comparison between ILUTP and IXYTP in Table 3 demonstrates robustness of the proposed structure-preserving preconditioners for different wave numbers, provided that a tight drop tolerance is used. That said, the better performance here, while encouraging, is accomplished at a high computational cost. The suboptimal performance of preconditioned iterative solvers based on incomplete factorizations for large wave numbers has been established in the literature [49]. Indeed, the Helmholtz problem is notoriously difficult.

Example (iii). 2D biharmonic equation Consider the fourth-order spectral differentiation matrix with homogeneous boundary conditions, (6). The coefficient matrix is the sum of a few sparse components and a dense cross derivative term, which makes it dense overall, and hence, using an iterative approach is not straightforward. We propose three different types of preconditioners for this system. The first pair are the ILU and IXY factors of the matrix corresponding to the squared spectral Poisson operator: if L and U are the ILU factors of the Poisson discrete operator, the ILU preconditioner of the biharmonic operator is defined as $(LU)^2$. We denote this matrix by G. We shall define the corresponding IXY preconditioner in an analogous manner. The second pair of preconditioners are defined as ILU and IXY factors of the sparse part of $\hat{\mathcal{A}}_{2DB}$,

$$C = (B \otimes I_{N-1}) + (I_{N-1} \otimes B).$$

The third pair of preconditioners are defined as

$$M = (B \otimes I_{N-1}) + (I_{N-1} \otimes B) + 2(D^2_{fd} \otimes D^2_{fd}),$$

where D^2_{fd} is the second-order finite difference scheme for Poisson operator with nodes at the collocation points. Note that all three pairs are sparse, including M, which contains the mixed derivative term.

We test our problems with GMRES, using the factors of ILU(0), IXY(0), ILUTP, and IXYTP, for the matrices G, C, and M. The density of the ILUTP factors for our selection of the drop tolerance is a bit higher than the density of the ILU(0) factors, but the number of iterations is significantly reduced. A similar observation can be made for IXYTP vs. IXY(0).

Equilibration [34, 50] is an effective way to improve the conditioning of linear systems. We use the row and column equilibration algorithm by Knight et al. [51], which preserves centrosymmetry. We have observed a significant reduction in condition numbers when we apply equilibration to linear systems involving spectral differentiation matrices.

In our numerical experiments, we consider $\hat{\mathcal{A}}_{2DB}$ with dimensions 324×324 and condition number 3.30×10^6. A linear system of this size would be considered too small to be solved using iterative solvers, but we believe that performing this small experiment is useful, nonetheless, to illustrate a few general points and in particular the excellent performance of the threshold-based incomplete factorization. The matrix is equilibrated to improves its condition number to 7.97×10^4. Without a preconditioner GMRES needs 185 iterations. We then run GMRES with the proposed preconditioners G, C and M. The numerical results indicate that of the three matrices tested, the IXY(0) and ILU(0) factors of M converge within the fewest number of iterations, followed by G and C. A comparison of convergence of GMRES, preconditioned by the IXY(0) and IXYTP factorizations of G, C, and M, is given in Fig. 5. GMRES preconditioned by the IXYTP factorization of M, with drop tolerance of 10^{-3}, needs seven iterations to achieve the same reduction in the relative residual. Notice that the IXY(0) factors require half the memory of ILU(0) factors.

Example (iv). 2D biharmonic equation with variable coefficients Next, we solve the linear system arising from applying spectral collocation to 2D variable-coefficient biharmonic equation with homogenous Dirichlet boundary conditions. Without

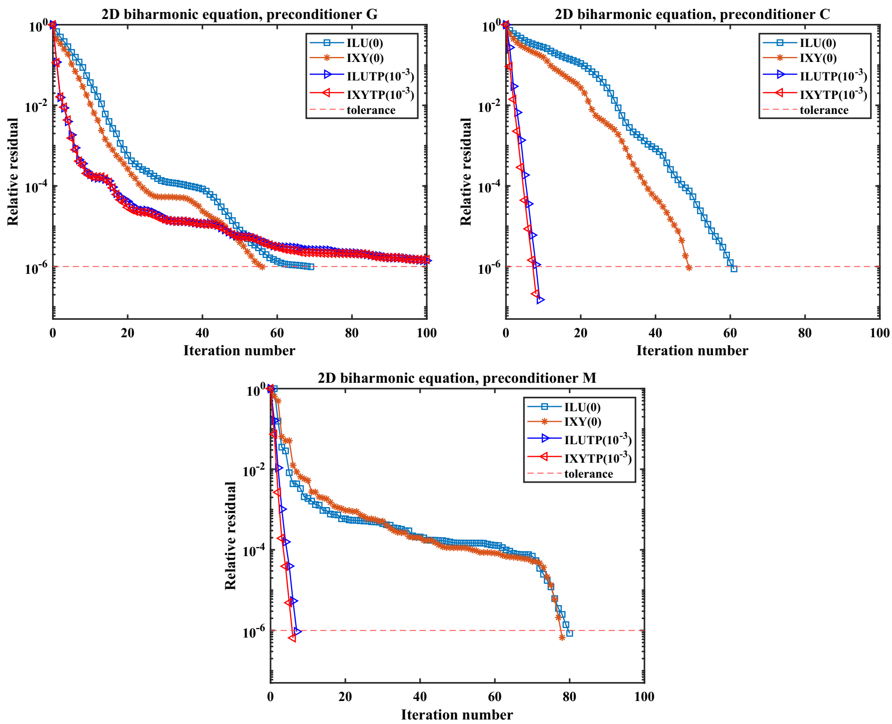

Fig. 5 Convergence of GMRES with three different pairs of preconditioners for the 2D biharmonic equation

considering the boundary conditions, the discretization leads to (14). The first preconditioner we consider is the sparse part of $\mathcal{A}_{2DBV}$

$$C = (D^2 \otimes I_{N+1})S(E \otimes I_{N+1}) + (I_{N+1} \otimes D^2)S(I_{N+1} \otimes E).$$

To implement the boundary conditions, we remove corresponding rows and columns to boundary conditions from this matrix. The modified matrix is denoted by $\hat{C}$. The second preconditioner for this system is defined as

$$M = \hat{C} + (D^2_{fd} \otimes I_{N-1})S(I_{N-1} \otimes D^2_{fd}) + (I_{N-1} \otimes D^2_{fd})S(D^2_{fd} \otimes I_{N-1}),$$

where D^2_{fd} is the second-order finite-difference scheme for Poisson operator with nodes at the collocation points.

Figure 6 shows the convergence of GMRES with the IXY(0) and IXYTP factors of C and M as preconditioners for the linear system with the spectral differentiation matrix arising from solving the 2D variable-coefficient biharmonic (13) with $a(x, y) = 1 + 10x^2y^2$. The results are compared to ILU(0) and ILUTP. We solve the system with a coefficient matrix of dimensions 400×400 and a condition number around 5.94×10^7, which after equilibration decreases to 1.0×10^4. GMRES without preconditioning needs around 224 iterations to achieve the desired reduction in relative residual. The IXYTP factorization M with drop tolerance 10^{-4} is computed, and the scheme converges within five iterations, while IXY(0) converges within 114 iterations to the same reduction in relative residual norm. The IXYTP factorization of C with drop tolerance 10^{-4} yields convergence within seven iterations, while IXY(0) converges in 58 iterations to the same reduction in relative residual norm.

In this example, as is the case in other examples, the static drop tolerance factorizations IXY(0) and ILU(0) are not competitive with the dynamic theshold-based factorizations IXYTP and ILUTP, and it is the latter that we are advocating for. Nonetheless, we include the results for the static patterns in order to illustrate the viability of IXY(0) in comparison with ILU(0).

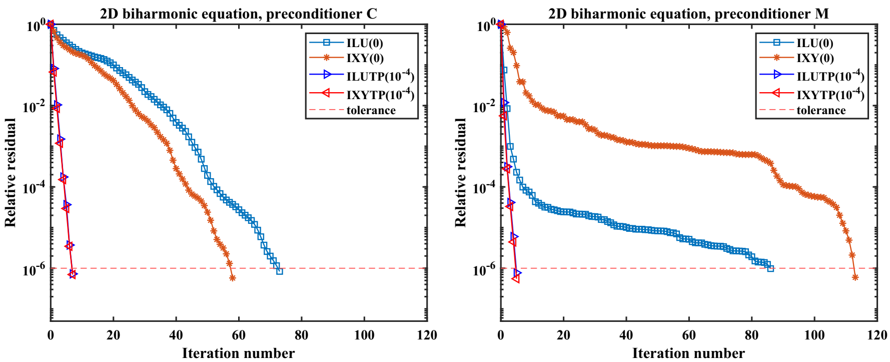

Fig. 6 Convergence of GMRES with proposed preconditioners C and M for the 2D variable-coefficient biharmonic equation

Example (v). Symmetric Legendre spectral differentiation matrix (SPD cases), Dirichlet, Neumann, and Robin boundary conditions The following examples concern symmetric positive definite linear systems. The top left corner of Fig. 7 examines the convergence of PCG preconditioned by IXX for the linear system given by (16). We compare IXX(0) and IXXT with the analogous incomplete Cholesky factorization. The matrix is 400 × 400. This is again a small example, and our main purpose here is to examine the effect of losing the centrosymmetry property. The density factor of the Cholesky factor is 9.79. Without preconditioning, PCG needs 131 iterations. The density factor of the IXXT factor is 2.10, and the density factor of IXX(0) is 1.9. With the IXXT factor as a preconditioner, PCG converges within five iterations, while with the IXX(0) factorization as a preconditioner, PCG converges in 18 iterations.

The top right corner of Fig. 7 shows the convergence results for the system given by the (19). The matrix is 400 × 400. The density factor of the Cholesky factor is 9.79. Without preconditioning, PCG needs 186 iterations. The density factor of the IXXT factor is 2.28, and the density factor of IXX(0) is 1.90. With the IXXT factor as a preconditioner, PCG converges within six iterations, while with the IXX(0) factorization as a preconditioner, PCG converges in 38 iterations.

In the bottom of Fig. 7, we show the results of applying the symmetric Legendre-Galerkin method for the Poisson equation with Robin boundary conditions. We choose

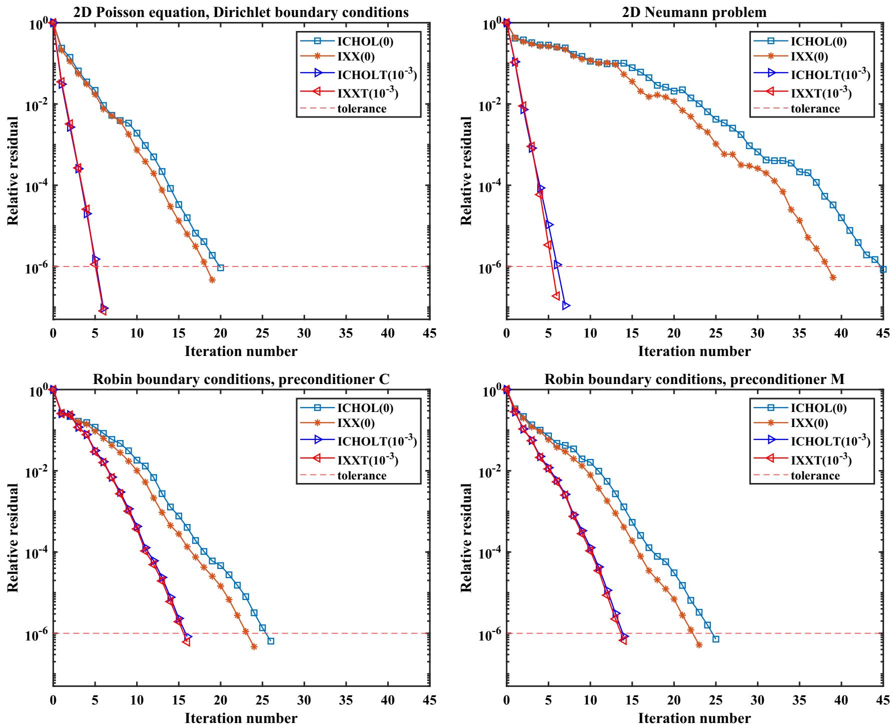

Fig. 7 Convergence of PCG with proposed preconditioners for the Poisson equation with Dirichlet/Robin boundary conditions and the Neumann problem

$a(x, y) = 1+\epsilon+x+y^2$ in (21), where $\epsilon = 10^{-5}$. The condition number of the matrix $\mathcal{A}_{2DPR}$ of size 400×400 is 5.81×10^3. The matrix is not centrosymmetric, and PCG with Cholesky factor as preconditioner converges in 112 iterations, where the density factor of the Cholesky factor is 9.79. The matrix $\mathcal{A}_{2DPR}$ is nearly centrosymmetric in the sense that it is centrosymmetric except along the diagonal. In the following, we propose two centrosymmetric approximations for the matrix $\mathcal{A}_{2DPR}$.

We first approximate $\mathcal{A}_{2DPR}$ with the matrix arising from spectral discretization of the same problem, where in the Robin boundary conditions, a is replaced by $\bar{a}$, the average of a,

$$\bar{a} = \frac{1}{\mid \partial\Omega \mid} \int_{\partial\Omega} a(x, y)dxdy.$$

The new matrix, which we refer as C, is centrosymmetric with the density factor of the IXXT factor with drop tolerance 10^{-3} is 2.00 and the density factor of IXX(0) is 1.90. With the IXXT factor as a preconditioner, PCG converges within 14 iterations, while with the IXX(0) factorization as a preconditioner, PCG converges in 23 iterations.

The second approximation is given by the centrosymmetric part of $\mathcal{A}$,

$$M = \frac{\mathcal{A} + J\mathcal{A}J}{2}.$$

PCG with IXX(0) and IXXT factors of this matrix converges in almost the same number of iterations as the former peconditioner C.

We see here that the loss of centrosymmetry has a negative effect on the performance of incomplete double-cone factorizations; however, they do stay competitive with their ILU counterparts.

Example (vi). 2D Helmholtz equation with Robin boundary condition In (24), we consider $a(x, y) = 2+x+y^2$. We set $N = 22$ in the spectral discretization and consider

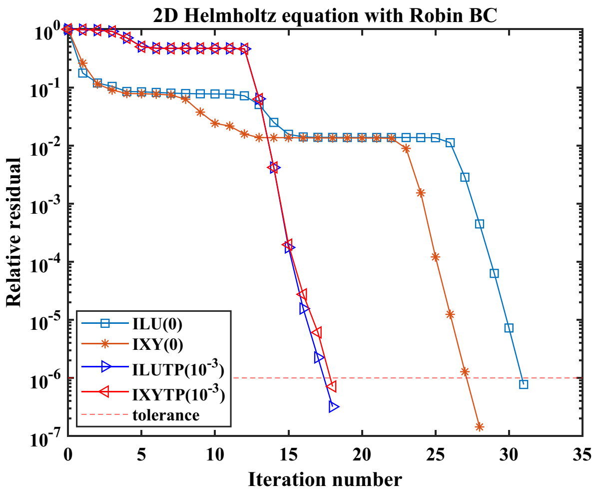

Fig. 8 Convergence of GMRES for the Helmholtz equation

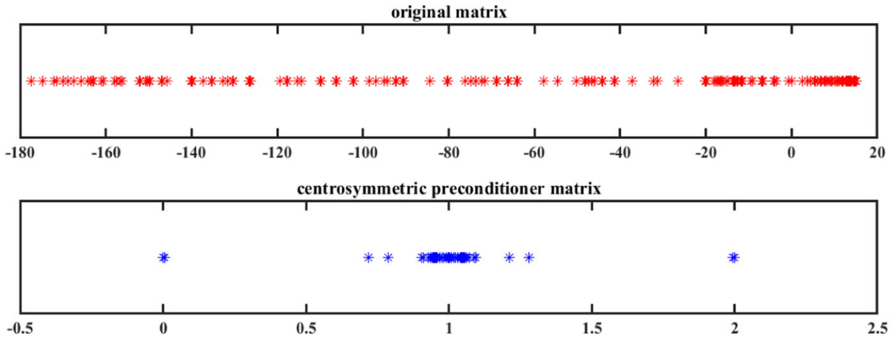

Fig. 9 Distribution of the eigenvalues of $\mathcal{A}_{2DHR}$ compared with distribution of the eigenvalues of the preconditioned system with the centrosymmetric part of the matrix

$k = 91.7907$, which is close to one of the eigenvalues of generalized eigenvalue problem. The condition number of the matrix $\mathcal{A}_{2DHR}$ given by similar (25) is 3.04×10^9. The matrix is nearly centrosymmetric. GMRES without preconditioner converges in 391 iterations, while with the ILU(0) and IXY(0) factors of the centrosymmetric part of the matrix as preconditioner, GMRES converges in 32 and 28 iterations, respectively. GMRES with ILUTP or IXYTP factors and drop tolerance 10^{-3} converges in 18 iterations in both cases, as shown in Fig. 8.

In Fig. 9, we compare the distribution of eigenvalues of $\mathcal{A}_{2DHR}$ with that of the system preconditioned by the centrosymmetric part of the matrix. As it shows, most of the eigenvalues of preconditioned system are positive and are bounded away from

Table 4 The number of GMRES iterations versus N, the number of collocation nodes for discretization. N_{nop} is the number of iterations of GMRES for solving the related linear system without using preconditioner, $N_{ilu(0)}$, $N_{ixy(0)}$, N_{ilutp} and N_{ixytp} are the number of iterations with using ILU(0), IXY(0), ILUTP and IXYTP factors of the matrix as preconditioners, respectively

$\mathcal{A}$	N	$\mathbf{N_{nop}}$	$\mathbf{N_{ilu(0)}}$	$\mathbf{N_{ixy(0)}}$	$\mathbf{N_{ilutp(10^{-3})}}$	$\mathbf{N_{ixytp(10^{-3})}}$
	12	59	12	11	3	3
2DP	16	95	15	14	4	4
	20	134	19	17	4	4
	12	93	15	14	5	4
3DP	16	157	18	18	5	5
	20	213	22	22	6	6
	12	84	30	23	7	7
2DB	14	113	40	31	7	7
precond C	18	185	61	49	9	8
	12	85	31	18	6	6
2DB	14	112	50	36	7	6
precond M	18	183	77	67	8	7

Table 5 Cost of computation (in seconds) for ILU(0) and IXY(0) solvers (timing for factorization is excluded). 3D Helmholtz problem is solved with wave number $k^2 = 1$

$\mathcal{A}$	N	Size ($\mathcal{A}$, 1)	$\mathbf{N_{ilu(0)}}$	$\mathbf{N_{ixy(0)}}$	Time $ilu(0)$	Time $ixy(0)$
3DP	11	1000	11	10	0.13	0.05
	21	8000	19	17	18.7	10.2
	31	27,000	26	24	338.4	187.7
3DH	11	1000	12	10	0.27	0.11
	21	8000	20	17	19.8	10.3
	31	27,000	27	25	349.6	162.11

0, with just one eigenvalue negative and close to zero; its value is -2.2×10^{-7}. This eigenvalue does not seem to have a seriously detrimental effect on the performance of the iterative scheme. For the original system, the eigenvalues are scattered between -177.39 and 15.19.

In Table 4, we compare the number of GMRES iterations versus N, the number of collocation nodes for discretization. The maximal value of N for each experiment conforms with the maximal value shown previously to obtain nearly full machine accuracy; this value is 20 for the first two experiments in the table and 18 for the last two. The table shows that preconditioning in this case successfully takes us in the direction of maintaining a higher level of scalability compared to the unpreconditioned case and that, altogether, our preconditioning approaches are robust with respect to the number of degrees of freedom. As illustrated in previous examples, the threshold-based incomplete factorization is particularly robust.

Finally, Table 5 provides a comparison of execution times for the GMRES solver using ILU(0) and IXY(0) factors as preconditioners. We use the matrix–vector product proposed by Fassbender and Ikramov [30] and the modified backward substitution introduced by Burnik [24] in GMRES. We also incorporate an implementation of the ILU algorithm given by Saad in [52] (Algorithm 10.2 in [46], Gaussian Elimination-IKJ Variant). With the current implementation and given examples, we report that the timing for the IXY(0) solver is almost two times faster than the ILU(0) solver. A more advanced implementation of ILU(0) and an improved version of IXY(0) that takes into account the centrosymmetry and sparsity pattern of the matrix would provide a more reliable indication of the time reduction achievable.

5 Concluding remarks

We have developed incomplete factorizations with a double-cone structure for centrosymmetric linear systems. This structure was identified and used previously for developing QR factorizations [24] for such systems, and we believe that the extension we propose to LU-type factorizations is useful. We have illustrated the merits of our approach on the important class of spectral differentiation matrices. Our IXYTP factorization provides a robust and cost-effective way to precondition centrosymmetric linear systems.

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Code availability The numerical code for solving the problems described in this paper is available at tinyurl.com/2uf3645d.

Declarations

Ethics approval Not applicable

Consent to participate Not applicable

Consent for publication Not applicable

Conflict of interest The authors declare no competing interests.

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