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Conjugate gradient for nonsingular saddle-point systems with a maximally rank-deficient leading block

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ABSTRACT

We consider iterative solvers for large, sparse, symmetric linear systems with a saddle-point structure. Since such systems are indefinite, the conjugate gradient (CG) method is not naturally designed for solving them. However, in the case of a maximally rank-deficient leading block, we prove that there are two sufficient conditions that allow for CG to be used. We show that the conditions are satisfied for a model time-harmonic Maxwell problem. To support our analysis, we present several numerical experiments for three-dimensional problems on complicated computational domains with constant and variable coefficients.

1. Introduction

Consider the regularized saddle-point system

$$\underbrace{\begin{pmatrix} A & B^T \\ B & -Q \end{pmatrix}}_{\mathcal{K}} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{m\times n}$ and $Q \in \mathbb{R}^{m\times m}$ with $m < n$. In many situations we have $Q = 0$, however for some PDE discretizations, using a symmetric positive semi-definite (SPSD) matrix $Q \neq 0$ can be utilized as a stabilization procedure. We focus our investigation on SPSD matrices A. In particular, we are interested in maximally rank-deficient leading blocks that still yields to a nonsingular block matrix, $\mathcal{K}$. For $Q = 0$, we require the following properties to ensure (1.1) is invertible:

$$\operatorname{rank}(A) = n - m, \quad \operatorname{rank}(B) = m, \quad \text{and} \quad \ker(A) \cap \ker(B) = \{0\}.$$

For $Q \neq 0$, the requirement on $\operatorname{rank}(B)$ can be relaxed.

In this paper, we derive two sufficient conditions that allow the use of the conjugate gradient (CG) method [1] to solve an indefinite saddle-point system with a maximally rank-deficient leading block, A. Our work builds on [2], where the authors developed an indefinite approximate inverse preconditioner for such problems. We expand this to consider the family of block diagonal and block triangular preconditioners from [3,4].

An outline of the rest of the paper follows. In Section 2, we give a comprehensive literature review for the use of CG for indefinite linear systems and outline our approach for this problem. In Section 3, we specifically construct the Krylov subspace and derive two sufficient conditions that allow CG to be used. In Section 4, we consider a null-space decoupling

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of (1.1). We analyze the spectral structure of the preconditioned matrices in Section 5. In Section 6, we show a series of three dimensional numerical experiments. Finally, we offer some concluding remarks in Section 7.

2. Literature review — conjugate gradient for indefinite linear systems

CG has been designed for symmetric positive definite (SPD) matrices. In particular, its derivation is based on minimizing the energy norm of the error, which is well defined only for SPD matrices. However, given the high effectiveness of the method, many extensions to other types of matrices have been considered. Applying CG to indefinite linear systems has been extensively investigated in the past 40 years, ranging from early methods in [5,6] in the 70s to more recent attempts such as [7] a few years ago. In the literature, some common approaches to the use of preconditioned or unpreconditioned CG for indefinite problems are:

1. Additively split the indefinite system into two parts, one being symmetric positive definite, and define a generalized CG algorithm;
2. Derive a nonstandard inner product with respect to which the preconditioned matrix is symmetric positive definite;
3. Preserve positivity of the eigenvalues of the preconditioned matrix.

In the pioneering work [5,6], the authors derive a generalized CG algorithm using a splitting approach. In [8], the Bramble–Pasciak CG algorithm is developed for regularized saddle point systems of the form (1.1). The authors use preconditioners of the form:

$$\begin{pmatrix} A_0 & 0 \\ B & I \end{pmatrix},$$

where A_0 is SPD. The preconditioned matrix is self-adjoint for the bilinear form defined by:

$$(\boldsymbol{x}, \boldsymbol{y})_{\mathcal{H}} = \boldsymbol{x}^T \mathcal{H} \boldsymbol{v} \quad \text{where} \quad \mathcal{H} = \begin{pmatrix} A - A_0 & 0 \\ 0 & I \end{pmatrix}.$$

We note that A_0 must be chosen such that $A - A_0$ is also SPD. The linear system associated with the preconditioned matrix can be solved by CG using the above defined inner product.

More recently, the authors in [9] showed that negating the second block row of a symmetric saddle-point matrix obtains the property that the new nonsymmetric saddle-point matrix,

$$\mathcal{K}_1 = \mathcal{J}\mathcal{K} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} A & B^T \\ B & -Q \end{pmatrix} = \begin{pmatrix} A & B^T \\ -B & Q \end{pmatrix},$$

has a spectrum that is entirely contained in the right half plane (all its eigenvalues have nonnegative real parts). The authors derive conditions by which $\mathcal{K}_1$ is diagonalizable with a real and positive spectrum. These are necessary and sufficient conditions that guarantee positive definiteness with respect to a certain bilinear form.

The authors in [10–12] show that for a certain class of constraint preconditioners of the form

$$\mathcal{P}_1 = \begin{pmatrix} G & B^T \\ B & -Q \end{pmatrix},$$

where G is SPD, the preconditioned matrix has positive eigenvalues. For example, for $G = \text{diag}(A)$, the authors in [11] proved that classical preconditioned CG is theoretically expected to converge if A is SPD. Thus, even though the preconditioner and saddle-point matrix are indefinite, CG can still be used. A more general framework for constraint preconditioners is offered in [13], where the authors derive projected preconditioned CG, and develop an effective way to apply it without explicitly forming the null-space of the matrix of constraints.

For more examples that consider CG for nonpositive definite matrices we refer the reader to [14], where the authors use a non-standard inner product in a similar way to [8]. Finally, see [7,15] for projected Krylov subspace methods.

In this work, we are interested in the class of regularized and unregularized saddle-point systems with a maximally rank-deficient leading block. The mathematical structure of this setting allows us to exploit the properties of the underlying Krylov subspace. For a preconditioner $\mathcal{P}$, the subspace given by:

$$\mathbb{K}_k(\mathcal{P}^{-1}\mathcal{K}, r_0) = \text{span}\{r_0,\ \mathcal{P}^{-1}\mathcal{K}\, r_0,\ \ldots,\ (\mathcal{P}^{-1}\mathcal{K})^{k-1}\, r_0\}, \tag{2.1}$$

where r_0 is preconditioned initial residual. If $\mathcal{K}$ and $\mathcal{P}$ are both SPD then clearly it is possible to apply CG. In this work $\mathcal{K}$ is indefinite, and thus, $\mathcal{P}^{-1}\mathcal{K}$ will not be SPD or even real positive. However, by explicitly forming the Krylov subspace and exploiting the block structure of $\mathcal{K}$ and $\mathcal{P}$, we derive two sufficient conditions for applying CG. Specifically, we simplify the first block vector of $(\mathcal{P}^{-1}\mathcal{K})^k r_0$ such that it can be expressed as a product of SPD and SPSD matrices and force the second block vector to 0. We can use CG even though the preconditioned matrix has both positive and negative eigenvalues and it is also structurally nonsymmetric.

3. Krylov subspace

In [3], the authors show that an ideal preconditioner for saddle-point systems of the form (1.1) with a maximally rank-deficient leading block is the augmented preconditioner:

$$\begin{pmatrix} A + B^T W^{-1} B & 0 \\ 0 & W \end{pmatrix}, \tag{3.1}$$

where W is an arbitrary symmetric positive definite matrix.

Our goal is to find conditions on an approximation X to the augmented term, $B^T W^{-1} B$, such that we can use preconditioned CG. We consider a preconditioner of the following form:

$$\mathcal{P} = \begin{pmatrix} A + X & 0 \\ 0 & W \end{pmatrix},$$

where X is chosen such that $A + X$ is SPD. It is possible to use CG to solve (1.1) when the preconditioned matrix $\mathcal{P}^{-1}\mathcal{K}$ is symmetrizable and its symmetrized version is positive definite. Considering a zero initial guess, the initial preconditioned residual is given by:

$$r_0 = \mathcal{P}^{-1} \begin{pmatrix} f \\ 0 \end{pmatrix} = \begin{pmatrix} (A + X)^{-1} f \\ 0 \end{pmatrix}. \tag{3.2}$$

To construct (2.1), an essential step is multiplication with the preconditioned matrix, which is given by:

$$\mathcal{P}^{-1}\mathcal{K} = \begin{pmatrix} A + X & 0 \\ 0 & W \end{pmatrix}^{-1} \begin{pmatrix} A & B^T \\ B & -Q \end{pmatrix} = \begin{pmatrix} (A + X)^{-1} A & (A + X)^{-1} B^T \\ W^{-1} B & -W^{-1} Q \end{pmatrix}.$$

Theorem 3.1. *Given a symmetric indefinite block 2×2 matrix and symmetric positive definite preconditioner*

$$\mathcal{K} = \begin{pmatrix} A & B^T \\ B & -Q \end{pmatrix} \quad \text{and} \quad \mathcal{P} = \begin{pmatrix} A + X & 0 \\ 0 & W \end{pmatrix},$$

assuming a zero initial guess, for the preconditioned residual r_0 given in (3.2), the resulting multiplications with the preconditioned matrices can be simplified as follows:

$$[\mathcal{P}^{-1}\mathcal{K}]^i r_0 = \begin{pmatrix} [(A + X)^{-1} A]^i (A + X)^{-1} f \\ 0 \end{pmatrix} \quad \text{for} \quad i = 0,\ 1,\ \ldots \tag{3.3}$$

as long as the following conditions hold:

$$C^T f = 0, \tag{3.4a}$$

$$AC = 0, \tag{3.4b}$$

where $C = (A + X)^{-1} B^T$.

Proof. The proof follows by induction. For $i = 0$ we have r_0, and for $i = 1$ we have

$$\mathcal{P}^{-1}\mathcal{K} r_0 = \begin{pmatrix} (A + X)^{-1} A (A + X)^{-1} f \\ W^{-1} B (A + X)^{-1} f \end{pmatrix}. \tag{3.5}$$

Thus by condition (3.4a) we see that (3.5) holds for $i = 1$. Now assuming

$$[\mathcal{P}^{-1}\mathcal{K}]^{i-1} r_0 = \begin{pmatrix} [(A + X)^{-1} A]^{i-1} (A + X)^{-1} f \\ 0 \end{pmatrix}, \tag{3.6}$$

it readily follows that

$$\begin{aligned} [\mathcal{P}^{-1}\mathcal{K}]^i r_0 &= [\mathcal{P}^{-1}\mathcal{K}][\mathcal{P}^{-1}\mathcal{K}]^{i-1} r_0 \\ &= \begin{pmatrix} (A + X)^{-1} A & (A + X)^{-1} B^T \\ W^{-1} B & -W^{-1} Q \end{pmatrix} \begin{pmatrix} [(A + X)^{-1} A]^{i-1} (A + X)^{-1} f \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} [(A + X)^{-1} A]^i (A + X)^{-1} f \\ W^{-1} B (A + X)^{-1} A [(A + X)^{-1} A]^{i-2} (A + X)^{-1} f \end{pmatrix} \\ &= \begin{pmatrix} [(A + X)^{-1} A]^i (A + X)^{-1} f \\ 0 \end{pmatrix}, \end{aligned}$$

where in the last step we used (3.4b). This completes the proof. □

From (3.4b) in Theorem 3.1 it readily follows that the null-space of A is defined as $C = (A+X)^{-1}B^T$. Multiplying by $A+X$ we can express the approximation X in terms of B^T and the null-space of A.

Corollary 3.1. *To satisfy (3.4b) in Theorem 3.1, X must be chosen such that:*

$$B^T = XC. \tag{3.7}$$

Remark 3.1. In Theorem 5.1, we considered left preconditioning. However, for right preconditioning the preconditioned matrix is $\mathcal{K}\mathcal{P}^{-1}$ and the associated Krylov subspace would be

$$\mathbb{K}_k(\mathcal{K}\mathcal{P}^{-1}, \tilde{r}_0) = \text{span}\{\tilde{r}_0,\ \mathcal{K}\mathcal{P}^{-1}\tilde{r}_0,\ \ldots,\ (\mathcal{K}\mathcal{P}^{-1})^{k-1}\tilde{r}_0\},$$

where $\tilde{r}_0 = \begin{pmatrix} f \\ 0 \end{pmatrix}$ is unpreconditioned initial residual for a zero initial guess. Using the conditions (3.4) one can prove a similar result to Theorem 3.1, that is:

$$[\mathcal{K}\mathcal{P}^{-1}]^i \tilde{r}_0 = \begin{pmatrix} [A(A+X)^{-1}]^i f \\ 0 \end{pmatrix} \quad \text{for } i = 0, 1, \ldots.$$

Thus, it is possible to use CG with left or right preconditioning.

Remark 3.2. The matrix X does not necessarily have to be positive definite, for the conditions in (3.4) to be satisfied. For example, if $X = B^T W^{-1} B$ then C is defined as:

$$C = (A + B^T W^{-1} B)^{-1} B^T. \tag{3.8}$$

In [2, Proposition 3.6] the authors show that if C is defined as in (3.8), then $AC = 0$. Thus, condition (3.4b) in Theorem 3.1 is automatically satisfied.

We now show that we are not restricted to the block diagonal preconditioner to enable the use of CG.

Proposition 3.1. *Consider the upper and lower triangular preconditioners:*

$$\mathcal{P}_U = \begin{pmatrix} A+X & B^T \\ 0 & W \end{pmatrix} \quad \text{and} \quad \mathcal{P}_L = \begin{pmatrix} A+X & 0 \\ B & W \end{pmatrix}. \tag{3.9}$$

Then

$$[\mathcal{P}_*^{-1}\mathcal{K}]^k r_0 = \begin{pmatrix} [(A+X)^{-1}A]^k (A+X)^{-1} f \\ 0 \end{pmatrix},$$

where $*$ denotes L or U, holds under the same conditions as in Theorem 3.1.

The proof follows by induction. The preconditioned matrices are

$$\begin{aligned} \mathcal{P}_U^{-1}\mathcal{K} &= \begin{pmatrix} (A+X)^{-1}A - (A+X)^{-1}B^T W^{-1} B & (A+X)^{-1}B^T \\ W^{-1}B & -W^{-1}Q \end{pmatrix}; \\ \mathcal{P}_L^{-1}\mathcal{K} &= \begin{pmatrix} (A+X)^{-1}A & (A+X)^{-1}B^T \\ W^{-1}B - W^{-1}B(A+X)^{-1}A & W^{-1}B(A+X)^{-1}B^T - W^{-1}Q \end{pmatrix}, \end{aligned}$$

and it follows that

$$[\mathcal{P}_*^{-1}\mathcal{K}]^k r_0 = \begin{pmatrix} [(A+X)^{-1}A]^k (A+X)^{-1} f \\ 0 \end{pmatrix},$$

where $*$ denotes L or U.

4. Null-space decoupling

Consider the saddle-point form of (1.1) with $Q = 0$. Since the null-space of A is of dimension m, there is matrix $C \in \mathbb{R}^{n\times m}$ whose columns form a linearly independent basis for the null-space of A. Using this null-space matrix, it is possible to decouple the saddle-point system (1.1) by multiplying the first block row with C^T to obtain:

$$C^T B^T v = C^T f.$$

The solution procedure for (1.1) becomes:

$$C^T B^T v = C^T f, \tag{4.1a}$$

$$Au = f - B^T v \quad \text{with} \quad Bu = 0. \tag{4.1b}$$

The solution of (4.1) is unique if and only if BC is nonsingular and A is positive definite on the null-space of B.

To aid discussion of the null-space decoupling, we introduce a Helmholtz-type decomposition similar to [2]. The intersection of the null-spaces of A and B is zero, thus:

$$\ker(A) \oplus \ker(B) = \mathbb{R}^n. \tag{4.2}$$

This decomposition provides key insights into the null-space decoupling of (1.1). Using (4.2) we write the primary variable solution

$$u = u_A + u_B$$

where $u_A \in \ker(A)$ and $u_B \in \ker(B)$.

Using [2, Proposition 3.6] and [2, Theorem 3.5], there exists a formulation of the null-space of A such that $W = BC$ is SPD, which allows the use of CG. From the Helmholtz-type decomposition (4.2), we can write (4.1b) as:

$$Au_B = f - B^T v \quad \text{with} \quad Bu_A = 0.$$

Since $u_A \in \ker(A)$ then $Bu_A \neq 0$ unless $u_A = 0$. Thus the decoupled system becomes

$$C^T B^T v = C^T f \quad \text{and} \quad Au_B = f - B^T v. \tag{4.3}$$

Since A is positive definite on the null-space of B, then it is possible to use a CG-type solver for the second equation in (4.3). In practice, since A is singular, one may apply a null-space method, which amounts to applying CG on:

$$Z^T A Z u_B = Z^T f \quad \text{where} \quad BZ = 0.$$

We note that a null-space matrix Z does not need to be explicitly constructed; see [13].

We conclude this section with a few comments for the case when $C^T f = 0$. In this setting ($\dim(\text{null}(A)) = m$), it is very common that the secondary variables, v, arise from a Lagrange multiplier formulation (1.1); see for example [16,17] for the mixed formulation of Maxwell's equations and [18] for norm minimization problems with equality constraints. Thus, the construction of f is often independent of the secondary variables, which leads to $C^T f = 0$ for these sorts of formulations. Thus, the solution to (4.1a) is zero and then the solution to (4.3) becomes:

$$Au_B = f. \tag{4.4}$$

Considering a preconditioner of the form $A + X$ for (4.4) would form the same block Krylov subspace defined in (3.3) where $v = 0$.

For a non-zero v, the discussion around (4.3) may indicate that the condition (3.4a) might be relaxed for the preconditioned saddle-point system.

5. Eigenvalue analysis

We now analyze the ideal forms of the preconditioner where we do not use the approximation X but rather the augmented term $B^T W^{-1} B$. We will consider the upper block triangular preconditioner:

$$\mathcal{P}_U = \begin{pmatrix} A + B^T W^{-1} B & B^T \\ 0 & W \end{pmatrix}.$$

Extension to block diagonal and block lower triangular can easily be done using the same techniques.

Theorem 5.1. *The preconditioned matrix $\mathcal{P}_U^{-1} K$ has eigenvalue $\lambda = 1$ with algebraic multiplicity $n - m$ and eigenvalue $\lambda = \frac{1 \pm \sqrt{5}}{2}$ with algebraic multiplicity $m - l$ for each eigenvalue, where $l = Dim(Null(A))Q$. The corresponding eigenpairs $(\lambda, \boldsymbol{x})$ are:*

$$\lambda = 1, \quad \boldsymbol{x} = (u_B, 0), \quad \text{and} \quad \lambda = \frac{1 \pm \sqrt{5}}{2}, \quad \boldsymbol{x} = (u_A, v_Q),$$

where $u_B \in Null(B)$, $u_A \in Null(A)$, and $v_Q \in Null(Q)$.

Proof. The corresponding generalized eigenvalue problem is given by:

$$\begin{pmatrix} A & B^T \\ B & -Q \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} A + B^T W^{-1} B & B^T \\ 0 & W \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \tag{5.1}$$

Assume λ is such that $(\lambda W + Q)$ is nonsingular. Such an assumption is valid, for example, for positive λ, because W and Q are SPD and SPSD, respectively. Substituting $v = (\lambda W + Q)^{-1} B u$ into the first block row of (5.1), we obtain:

$$(1 - \lambda) Au + (1 - \lambda) B^T (\lambda W + Q)^{-1} B u = \lambda B^T W^{-1} B u.$$

From this, it follows immediately that if $u \in \text{Null}(B)$ then $\lambda = 1$ is an eigenvalue.

Table 1
Eigenpairs and algebraic multiplicities for the preconditioned matrices $\mathcal{P}_D^{-1}K$ and $\mathcal{P}_L^{-1}K$. We use the notation $u_B \in \text{Null}(B)$, $u_A \in \text{Null}(A)$, $v_Q \in \text{Null}(Q)$, and $l = \text{Dim}(\text{Null}(Q))$.

Preconditioned matrix	Eigenvalue	Eigenvector	Algebraic multiplicity
$\mathcal{P}_D^{-1}K$	1	(u, v_Q)	$n-l$
$\mathcal{P}_D^{-1}K$	-1	(u_A, v_Q)	$m-l$
$\mathcal{P}_L^{-1}K$	1	$(u_B, 0)$	$n-m$
$\mathcal{P}_L^{-1}K$	$\frac{1+\sqrt{5}}{2}$	(u_A, v_Q)	$m-l$
$\mathcal{P}_L^{-1}K$	$\frac{1-\sqrt{5}}{2}$	(u_A, v_Q)	$m-l$

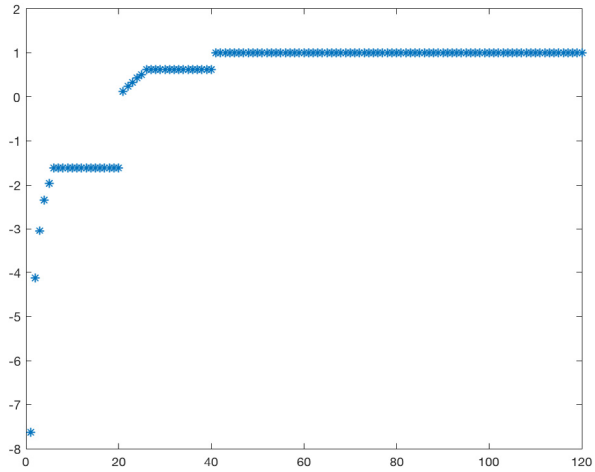

Fig. 1. Eigenvalue distribution of the preconditioned matrix $\mathcal{P}_U^{-1}K$ using randomly generated blocks with $n = 100$, $m = 20$, and $l = 5$.

Now, assume that $\lambda \neq 1$ and $Bu \neq 0$. Substituting $Bu = (\lambda W + Q)v$ into (5.1) gives:

$$(\lambda - 1)Au + (\lambda^2 + \lambda - 1)B^T v + \lambda B^T W^{-1} Q v = 0.$$

Thus by setting $u \in \text{Null}(A)$, and $v \in \text{Null}(Q)$, we have $\lambda = \frac{1\pm\sqrt{5}}{2}$. □

From Theorem 5.1 it follows that if $Q = 0$, we have the full spectrum of the preconditioned matrix, with just three distinct eigenvalues that have high algebraic multiplicities.

Corollary 5.1. *For the non-regularized saddle-point form of (1.1), with $Q = 0$, $\mathcal{P}_U^{-1}K$ has eigenvalue $\lambda = 1$ with algebraic multiplicity $n - m$ and eigenvalues $\lambda_\pm = \frac{1\pm\sqrt{5}}{2}$ with algebraic multiplicities m.*

Proposition 5.1, given below, outlines the algebraic multiplicities of eigenvalues and their corresponding eigenvectors for block diagonal and block lower triangular preconditioners. The full eigenvalue analysis for these preconditioners is omitted since it is very similar to what we show in Theorem 5.1.

Proposition 5.1. *Consider the preconditioners*

$$\mathcal{P}_D = \begin{pmatrix} A + B^T W^{-1} B & 0 \\ 0 & W \end{pmatrix} \quad \text{and} \quad \mathcal{P}_L = \begin{pmatrix} A + B^T W^{-1} B & 0 \\ B & W \end{pmatrix}.$$

Then the eigenpairs and algebraic multiplicities of the preconditioned matrices are given in Table 1.

In Fig. 1 we show an example of the eigenvalue distribution of the preconditioned matrix.

6. Numerical experiments

In this section we use the time-harmonic Maxwell equation in mixed form [4,19] to illustrate our findings. The continuous problem is given as follows:

$$\begin{aligned} \nabla \times \nu \nabla \times \boldsymbol{b} + \nabla r &= \boldsymbol{f} \quad \text{in } \Omega \\ \nabla \cdot \boldsymbol{b} &= 0 \quad \text{in } \Omega, \end{aligned} \tag{6.1}$$

Table 2
Krylov solver test: time and iteration results for using one iterations of the preconditioner with FCG, MINRES and GMRES. The viscosity for these tests is $\nu = 1e{-}2$.

		FCG			MINRES			GMRES		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
3	4913	0.06	14	2.4/1.4	0.07	13	3.0/1.9	0.07	12	3.0/1.9
4	35,937	0.70	14	2.7/1.7	0.72	13	3.6/1.9	0.78	13	3.5/2.1
5	274,625	5.82	13	3.1/2.2	7.42	14	3.9/2.9	7.57	13	3.9/2.8
6	2,146,689	61.78	15	3.3/2.1	60.36	12	4.2/2.8	78.06	14	4.2/2.9
7	16,974,593	580.22	14	3.9/2.5	601.85	13	4.5/2.9	712.28	13	4.9/2.9

where $\boldsymbol{b}$ is the magnetic field and r is the Lagrange multiplier associated with the divergence constraint on the magnetic field. The constant ν is the magnetic viscosity. This model is well understood and gives rise, upon finite element discretization, to a symmetric system; see [4,20]. It also arises in coupled electromagnetic flows such as magnetohydrodynamics; see [21,22] and the references therein.

We consider a finite element discretization of (6.1) which uses Nédélec elements for the magnetic field and nodal elements for the multiplier variable. See [4,20] for more details. Upon discretization, A, B and B^T are defined to be the discrete curl–curl, magnetic gradient and magnetic divergence operators, respectively. Thus, the null-space of A is the discrete gradient operator and has dimension m. The resulting discretization of (6.1) falls into the class of saddle-point systems with a maximally rank-deficient leading block. We note that a sparse construction of the discrete gradient operator for first order Nédélec elements is possible [20, Section 2].

In [4] it was shown that the vector mass matrix and scalar Laplacian are appropriate choices for X and W, respectively. We now show that for these choices, the conditions (3.4a)–(3.4b) in Theorem 3.1 hold. In [4, Proposition 2.2] the authors prove the identity

$$B^T = XC,$$

where we recall that B^T and C are the magnetic divergence and discrete gradient operators, respectively. Thus, by Corollary 3.1, (3.4b) holds. Typically, the right-hand-side is divergence-free for physical applications; see [16,22]. Since C is the null-space operator of the curl–curl matrix, C^T is a discrete divergence operator. Hence, the divergence-free condition (3.4a) holds.

Therefore, for the Maxwell problem of the form (6.1) the conditions (3.4a)–(3.4b) hold and enable the use of CG with either a block diagonal, upper or lower block triangular preconditioner.

Let us consider a 3D example with a smooth solution on $\Omega = [0, 1]^3$. The analytical solution is set to be

$$\begin{aligned} \boldsymbol{b}(x, y, z) &= \begin{pmatrix} -\exp(x+y+z)\sin(y) + \exp(x+y+z)\sin(z) \\ xy\exp(x+y+z) - yz\exp(x+y+z) \\ -\exp(x+y+z)\sin(x) + \exp(x+y+z)\sin(y) \end{pmatrix} \\ r(x, y, z) &= 0. \end{aligned} \tag{6.2}$$

Then the source terms $\boldsymbol{f}$ in (6.1) and inhomogeneous boundary conditions are defined from the analytical solution. By construction, we have ensured that the right-hand-side is divergence-free. We use this setup as a basis for all numerical experiments and outline any alterations (e.g., the domain or multiplier variable) we make for the specific example.

In each experiment we use a tolerance of $1e{-}6$ for the outer Flexible CG (FCG) iteration [23]. For the inner solves ($A+X$ and W), we use the auxiliary space preconditioner of [24]. This entails a CG solve for $A+X$ and W with a tolerance of $1e{-}3$ for each. In the subsequent tables we use the following notation:

- ℓ: mesh level;
- DoFs: number of degrees of freedom for Magnetic field plus the multiplier variables;
- Time: solution time;
- it: number of outer iterations;
- it_1: number of inner CG/Auxiliary Space iterations for $A + X$;
- it_2: number of inner CG/Auxiliary Space iterations for W.

6.1. Krylov subspace solver test

The first numerical experiment we consider is to test the robustness and performance of FCG compared to other Krylov subspace methods. We set this inner tolerance to be $1e{-}4$ and test against MINRES [25] and GMRES [26]. The results are shown in Table 2. We observe that the iteration counts are similar for all three methods tested, and FCG is slightly superior in terms of computational time. Given that the cost of single iterations is lower for FCG compared to MINRES, and given that the memory consumption of FCG is significantly lower than that of GMRES, we conclude that FCG is the most effective method of the three, although not by a significant margin.

Table 3
Block preconditioner test: time and iteration results using the block diagonal ($\mathcal{P}$), block upper triangular ($\mathcal{P}_U$) and block lower triangular ($\mathcal{P}_L$) preconditioners with $\nu = 1e{-}2$.

		$\mathcal{P}$			$\mathcal{P}_U$			$\mathcal{P}_L$		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
2	729	0.01	12	1.8/1.0	0.01	13	1.7/1.1	0.01	13	1.7/1.1
3	4,913	0.07	14	2.3/1.4	0.05	13	2.2/1.5	0.05	13	2.1/1.6
4	35,937	0.64	14	2.5/1.7	0.57	14	2.5/1.7	0.56	14	2.5/1.7
5	274,625	5.95	14	2.7/1.7	6.11	16	2.6/1.6	5.41	14	2.6/1.8
6	2,146,689	56.92	14	2.9/1.8	60.92	16	2.9/1.7	59.89	16	2.9/1.7
7	16,974,593	574.34	14	3.3/2.3	589.14	16	3.2/2.2	569.86	16	3.2/2.1

Table 4
Divergence-free vs. non-divergence-free right-hand-side: time and iteration results using the block diagonal preconditioner, $\mathcal{P}$, for divergence and non-divergence free right-hand-sides with $\nu = 1e{-}2$.

		Divergence Free			Non-divergence Free		
l	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2
2	729	0.01	12	1.5/0.9	0.01	12	1.5/0.9
3	4,913	0.06	14	2.3/1.4	0.06	14	2.3/1.4
4	35,937	0.64	14	2.5/1.7	0.64	14	2.5/1.7
5	274,625	7.41	14	2.7/1.7	7.41	14	2.7/1.7
6	2,146,689	55.02	14	2.9/1.8	55.02	14	2.9/1.8
7	16,974,593	544.91	14	3.3/2.3	644.91	14	3.3/2.6

6.2. Block preconditioner test

Let us now consider preconditioned CG with diagonal and upper/lower triangular preconditioners. The results are given in Table 3. From Theorem 3.1 and Proposition 3.1, we have shown that the Krylov subspace for both the diagonal and block triangular preconditioners are same. Thus we would expect the number of iterations for FCG to converge to be identical. From the table, we can see that the block diagonal preconditioner preforms slightly better with respect to the outer FCG iterations. We have shown that the preconditioner with the exact augmented term ($X = B^T W^{-1} B$) has two distinct eigenvalues for the preconditioned matrix, whereas for the block triangular preconditioner we have three distinct eigenvalues for the preconditioned matrix. This may explain the slight difference in performance.

6.3. Divergence and non-divergence free right-hand-side

Let us now consider divergence and non-divergence free right-hand-sides. The results are given in Table 4. We observe that there is almost no difference in the iteration results between the divergence and non-divergence free right-hand-side solution. This shows that even though our analysis requires a divergence-free right-hand side, in practice the solver is robust with respect to right-hand side vectors that violate this condition. We do not have a theoretical justification for this. If the right-hand-side is not divergence free then term (3.5) does not vanish and the construction of the Krylov subspace is significantly more involved. In that case, there is no easy way to discern algebraic structure and proceed with deriving results such as (3.3) in Theorem 3.1. However, in Section 4 we showed that it is possible to decouple such saddle point systems into two SPD linear systems, and those systems can be solved with CG even if the divergence constraint is not satisfied. Therefore, we suspect that the divergence-free condition can be relaxed in practice.

6.4. Variable coefficients

We now let the magnetic viscosity be defined as:

$$\nu = \begin{cases} 1/a & \text{if } x < 0.5 \text{ and } y < 0.5 \text{ and } z < 0.5, \\ 1/2a & \text{if } x > 0.5 \text{ and } y < 0.5 \text{ and } z < 0.5, \\ 1/3a & \text{if } x < 0.5 \text{ and } y > 0.5 \text{ and } z < 0.5, \\ 1/4a & \text{if } x > 0.5 \text{ and } y > 0.5 \text{ and } z < 0.5, \\ 1/5a & \text{if } x < 0.5 \text{ and } y < 0.5 \text{ and } z > 0.5, \\ 1/6a & \text{if } x > 0.5 \text{ and } y < 0.5 \text{ and } z > 0.5, \\ 1/7a & \text{if } x < 0.5 \text{ and } y > 0.5 \text{ and } z > 0.5, \\ 1/8a & \text{otherwise,} \end{cases}$$

where a is a constant. Tables 5 and 6 show iteration and timing results for the block diagonal and triangular preconditioners for various values of a. We can see from Table 5 that as a increases then the number of outer FCG iterations increase but the inner Auxiliary Space iterations seem relatively constant, with only a slight increase going through the

Table 5
Variable coefficients: time and iteration results using the block diagonal preconditioner, $\mathcal{P}$, for various different values of a.

		$a = 10$			$a = 100$			$a = 1000$		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
2	729	0.01	14	1.9/0.9	0.02	32	1.4/0.9	0.06	71	0.9/0.6
3	4,913	0.10	15	2.3/1.5	0.18	38	2.0/1.3	0.36	98	1.4/1.2
4	35,937	0.71	15	2.8/1.7	1.51	39	2.2/1.6	3.23	110	1.8/1.5
5	274,625	6.46	15	3.0/1.9	13.96	40	2.6/1.7	34.18	116	2.2/1.6
6	2,146,689	63.63	15	3.8/1.9	132.51	40	2.9/1.8	328.45	116	2.4/1.8
7	16,974,593	581.03	15	3.9/2.2	1306.93	40	3.3/2.3	3267.59	122	2.7/2.3

Table 6
Variable coefficients: time and iteration results using the block diagonal and triangular preconditioners for $a = 100$.

		$\mathcal{P}$			$\mathcal{P}_U$			$\mathcal{P}_L$		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
2	729	0.02	32	1.4/0.9	0.01	32	1.3/0.8	0.02	34	1.3/0.9
3	4,913	0.18	38	2.0/1.3	0.15	38	1.9/1.3	0.14	38	1.8/1.3
4	35,937	1.51	39	2.2/1.6	1.43	39	2.3/1.6	1.43	40	2.1/1.6
5	274,625	13.96	40	2.6/1.7	14.62	41	2.6/1.7	14.64	41	2.4/1.7
6	2,146,689	132.51	40	2.9/1.8	147.63	41	3.0/1.8	150.59	43	2.9/1.8
7	16,974,593	1306.93	40	3.3/2.3	1557.95	42	3.4/2.4	1572.68	44	3.2/2.3

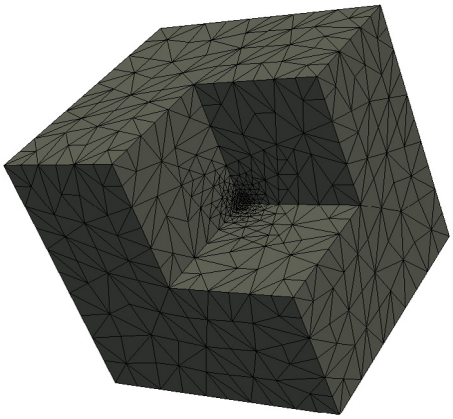

Fig. 2. Fichera corner domain for mesh level, $\ell = 1$.

levels. For $a = 10$ or 100 the outer FCG iterations remain approximately constant but for $a = 1000$ the outer iterations start to degrade slightly. Table 6 shows the iteration and timing comparisons between the block diagonal and triangular preconditioners for $a = 100$. Again, we see that the outer iteration FCG iterations appear to be slightly better for the block diagonal preconditioner than the block triangular versions. We also note that solve time for the triangular versions are higher, especially for the larger mesh levels. This is due to the extra multiplications with B or B^T for the block triangular preconditioners.

6.5. Fichera corner problem

For our next numerical illustration, we consider the same exact solution in (6.2), however the domain will be a cube missing a corner. That is, the domain is $\Omega = (-1, 1)^3/[0, 1) \times [0, 1) \times [0, 1)$ with local refinement in the corner. A visualization of this domain is given in Fig. 2. We investigate how the magnetic viscosity effects the iterations on such a domain. Table 7 presents the results. The table shows that as the magnetic viscosity decreases the number of outer FCG iterations increase. As with the previous example, inner Auxiliary Space iterations appear to be scalable.

6.6. Gear domain

For our final experiment, we consider the same exact solution in (6.2) however with a quasi-uniform 3-dimensional gear as the domain. The domain is bounded in $\Omega = [-1, 1] \times [-1, 1] \times [0, -0.2]$. A visualization of this domain is given in Fig. 3.

Table 7
Fichera corner: time and iteration results using the block diagonal preconditioner, $\mathcal{P}$, for various different values of ν.

		ν =1e−1			ν =1e−2			ν =1e−3		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
1	14,636	0.41	13	3.8/2.0	0.73	31	3.7/2.3	1.69	80	3.9/2.6
2	111,315	3.84	13	4.4/2.5	7.23	31	4.2/3.0	17.01	81	4.5/3.4
3	869,397	45.74	13	5.9/2.7	85.37	32	5.2/3.3	181.89	72	5.0/3.6
4	6,874,601	614.06	15	8.1/3.4	1027.89	31	6.4/3.7	2248.88	69	6.4/4.2

Table 8
Gear domain: time and iteration results using the block diagonal preconditioner, $\mathcal{P}$, for various different values of ν.

		ν =1e−1			ν =1e−2			ν =1e−3		
ℓ	DoFs	Time	it	it_1/it_2	Time	it	it_1/it_2	Time	it	it_1/it_2
6	16,680	0.23	8	2.2/1.4	0.41	19	2.6/1.5	0.83	42	2.3/1.4
7	106,940	2.62	10	4.0/2.0	4.70	21	4.2/2.5	9.08	44	3.0/2.3
8	774,871	69.85	10	8.8/2.5	77.25	17	5.2/3.2	173.12	46	4.4/3.7
9	5,950,932	1387.91	10	17.2/4.5	1554.78	18	10.2/5.1	3227.96	48	7.8/6.0

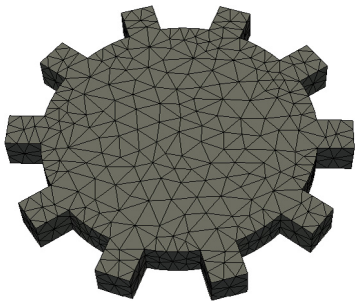

Fig. 3. Gear domain for mesh level, $\ell = 5$.

Table 8 shows iteration and timing results for the constant coefficients. From the table we can see that as we decrease ν the outer FCG iterations increase slightly but appear to remain constant with respect to the mesh size. For this example, the inner iterations are starting to increase slightly more every mesh level. However, the number of iterations are relatively small and still give a fast solution procedure.

7. Conclusions

In this work, we have proven that there are two sufficient conditions which enable the use of the conjugate gradient method (CG) for a nonsingular saddle-point system with a maximally rank-deficient leading block. We have shown that these conditions are satisfied by the properties of the mixed time-harmonic Maxwell problem.

We have presented several non-trivial large-scale three-dimensional numerical experiments of the Maxwell problem with variable coefficients on complicated domains.

We have also shown that for block triangular preconditioners, which are nonsymmetric, it is still possible to use CG under the same conditions as the block diagonal preconditioner.

CG is known to be the method of choice for symmetric positive definite matrices. The memory requirements are modest and the cost of iterations is lower compared to its competitors. It is thus beneficial to have CG as an option in nonsymmetric settings, under the conditions we have stated. For the Maxwell problem considered here, the block diagonal preconditioner appears to be slightly more effective than the triangular versions.

The condition (3.7) in Corollary 3.1 is rather restrictive and it would be desirable to relax it. Approaches such as the one in [2, Proposition 4.3] may be used.

Finally, the maximal rank deficiency of the leading block is key for our numerical and theoretical results. However, it is rather restrictive and it would be desirable to be able to apply CG for a wider class of problems; see for example [2, Section 5.2]

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