# An augmented Lagrangian-based preconditioning technique for a class of block three-by-three linear systems

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#### Abstract

We propose an augmented Lagrangian-based preconditioner to accelerate the convergence of Krylov subspace methods applied to linear systems of equations with a block three-by-three structure such as those arising from mixed finite element discretizations of the coupled Stokes-Darcy flow problem. We analyze the spectrum of the preconditioned matrix and we show how the new preconditioner can be efficiently applied. Numerical experiments are reported to illustrate the effectiveness of the preconditioner in conjunction with flexible GMRES for solving linear systems of equations arising from a 3D test problem.

*Keywords:* Krylov subspace methods; Preconditioning techniques; Spectral analysis; Coupled Stokes-Darcy flow problem.

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### 1. Introduction

Consider the following  $(n + m + p) \times (n + m + p)$  linear system of equations:

$$\mathcal{A}u = \begin{bmatrix} A_{11} & A_{12} & 0\\ A_{21} & A_{22} & B^T\\ 0 & B & 0 \end{bmatrix} \begin{bmatrix} u_1\\ u_2\\ u_3 \end{bmatrix} = \begin{bmatrix} b_1\\ b_2\\ b_3 \end{bmatrix} = b,$$
(1.1)

where  $A_{11}$  and  $A_{22}$  are both symmetric positive definite (SPD),  $A_{21} = -A_{12}^T$  and *B* has full row rank. In this paper, we are especially interested in the case where the above system corresponds to inf-sup stable mixed finite element discretizations of the coupled Stokes-Darcy flow problem; see [2, 3] for further details. Krylov subspace methods (such as GMRES) in conjunction with suitable preconditioners are frequently the method of choice for computing approximate solutions of such linear systems of equations; see [1, 2, 3] and the references therein.

In [1], first, problem (1.1) is reformulated as the equivalent *augmented* system  $\bar{A}u = \bar{b}$ , where

$$\bar{\mathcal{A}} = \begin{bmatrix} A_{11} & A_{12} & 0\\ A_{21} & A_{22} + \gamma B^T Q^{-1} B & B^T\\ 0 & B & 0 \end{bmatrix},$$
(1.2)

and  $\bar{b} = (b_1; b_2 + \gamma B^T Q^{-1} b_3; b_3)$ , with Q being an arbitrary SPD matrix and  $\gamma > 0$  a user-defined parameter. Then, the following preconditioner is proposed:

$$\mathcal{P}_{\gamma} = \begin{bmatrix} A_{11} & A_{12} & 0\\ 0 & A_{22} + \gamma B^T Q^{-1} B & B^T\\ 0 & 0 & -\frac{1}{\gamma} Q \end{bmatrix}.$$

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In practice, this preconditioner is applied inexactly by means of inner iterations and thus is used with Flexible GMRES (FGMRES) [5]. It was observed in [1] that FGMRES with the inexact augmented Lagrangianbased preconditioner  $\mathcal{P}_{\gamma}$  exhibits faster convergence for larger values of  $\gamma$ . However, for large  $\gamma$  the total timings increase due to the fact that the condition number of the block  $A_{22} + \gamma B^T Q^{-1}B$  goes up as  $\gamma$  increases. Hence, the conjugate gradient (CG) method used for solving subsystems with coefficient matrix  $A_{22} + \gamma B^T Q^{-1}B$  needs to be applied with a preconditioner. Explicitly forming  $A_{22} + \gamma B^T Q^{-1}B$  to compute an incomplete Cholesky factorization leads to a considerably less sparse matrix and superlinear growth in the fill-in in the incomplete factors, and thus to more expensive preconditioned CG (PCG) iterations; for further details see [1, Table 2].

In this paper, we introduce a new class of preconditioners for  $\overline{A}$  given as follows:

$$\mathcal{P}_{\gamma,\alpha} = \begin{bmatrix} A_{11} & A_{12} & 0\\ 0 & A_{22} + \gamma B^T Q^{-1} B & (1 - \gamma \alpha^{-1}) B^T\\ 0 & B & -\alpha^{-1} Q \end{bmatrix}$$
(1.3)

where  $\alpha$  and  $\gamma$  are prescribed positive parameters such that  $\alpha \geq \gamma$ . As shown below, this form of preconditioning allows us to avoid the requirement of forming the augmented block  $A_{22} + \gamma B^T Q^{-1}B$ , which makes it possible to work with large values of  $\gamma$ . It is also highly effective in reducing the number of FGMRES iterations.

The rest of paper is organized as follows. In section 2, we derive some bounds for the eigenvalues of the preconditioned matrix  $\bar{\mathcal{AP}}_{\gamma,\alpha}^{-1}$ . Numerical results are presented in section 3 which illustrate the effectiveness of the proposed preconditioner in conjunction with FGMRES in terms of both the number of iterations and the CPU time. Section 4 concludes the paper.

**Notations.** Given a square matrix A, the set of all eigenvalues (spectrum) of A is denoted by  $\sigma(A)$ . When the spectrum of A is real, we use  $\lambda_{\min}(A)$  and  $\lambda_{\max}(A)$  to respectively denote its minimum and maximum eigenvalues. When A is symmetric positive (semi)definite, we write  $A \succ 0$  ( $A \succeq 0$ ). In addition, for two given matrices A and B, the relation  $A \succ B$  ( $A \succeq B$ ) means  $A - B \succ 0$  ( $A - B \succeq 0$ ). Finally, for vectors x, y and z of dimensions n, m and p, (x; y; z) will denote a column vector of dimension n + m + p. Throughout the paper, I will denote the identity matrix (the size of which will be clear from the context).

#### 2. Main results

with

In this section, we first obtain some bounds for the eigenvalues of  $\mathcal{P}_{\gamma,\alpha}^{-1}\overline{\mathcal{A}}$  (which coincide with those of  $\overline{\mathcal{A}}\mathcal{P}_{\gamma,\alpha}^{-1}$ ; recall that only right preconditioning is allowed with FGMRES ). We show that using large values of  $\alpha$  leads to a well clustered eigenvalue distribution for the preconditioned matrix. Then we explain how the preconditioner can be efficiently implemented.

**Theorem 2.1.** Let  $\bar{\mathcal{A}}$  and  $\mathcal{P}_{\gamma,\alpha}$  be respectively defined by (1.2) and (1.3). The eigenvalues of  $\sigma(\mathcal{P}_{\gamma,\alpha}^{-1}\bar{\mathcal{A}})$  are all real and positive. More precisely, for an arbitrary  $\lambda \in \sigma(\mathcal{P}_{\gamma,\alpha}^{-1}\bar{\mathcal{A}})$ , we have

$$\begin{aligned} \frac{\xi^2 \alpha \lambda_{\min}(Q)}{\lambda_{\max}(Q)((\lambda_{\max}(A_{22}) + \lambda_{\max}(A_{12}^T A_{11}^{-1} A_{12}))\lambda_{\min}(Q) + 2\alpha \|B\|_2^2)} &\leq \lambda < 2 + \frac{\lambda_{\max}(A_{12}^T A_{11}^{-1} A_{12})}{\lambda_{\min}(A_{22})}\\ \xi &= \min\left\{\|By\|_2 \mid y \notin \operatorname{Ker}(B), \ y^*y = 1\right\}.\end{aligned}$$

*Proof.* For simplicity, we set  $\bar{A}_{22} = A_{22} + \gamma B^T Q^{-1} B$ . Let  $\lambda$  and (x; y; z) be an arbitrary eigenpair of  $\mathcal{P}_{\gamma,\alpha}^{-1} \bar{\mathcal{A}}$ . Therefore, we have

$$A_{11}x + A_{12}y = \lambda(A_{11}x + A_{12}y) \tag{2.1a}$$

$$A_{21}x + \bar{A}_{22}y + B^T z = \lambda(\bar{A}_{22}y + (1 - \gamma \alpha^{-1})B^T z)$$
(2.1b)

 $By = \lambda (By - \alpha^{-1}Qz) \tag{2.1c}$ 

From Eq. (2.1a), we deduce that either  $\lambda = 1$  or  $x = -A_{11}^{-1}A_{12}y$ . In particular, one can verify that  $\lambda = 1$  belongs to the spectrum of  $\mathcal{P}_{\gamma,\alpha}^{-1}\bar{\mathcal{A}}$  with a corresponding eigenvector of the form (x; y; 0) provided that x and y are not simultaneously zero and that  $x \in \text{Ker}(A_{21})$ .

In the rest of the proof, we assume that  $\lambda \neq 1$ . Notice that if  $y \in \text{Ker}(B)$ , then Eq. (2.1c) implies that z is the zero vector. Hence, from (2.1b), one can conclude that

$$\lambda = 1 + \frac{y^* A_{12}^T A_{11}^{-1} A_{12} y}{y^* \bar{A}_{22} y} = 1 + \frac{y^* A_{12}^T A_{11}^{-1} A_{12} y}{y^* A_{22} y}.$$
(2.2)

In the sequel, without loss of generality, we may assume that  $y \notin \text{Ker}(B)$  and  $y^*y = 1$ . Since  $\lambda \neq 1$ , from (2.1c), we further obtain

$$z = \alpha \left(\frac{\lambda - 1}{\lambda}\right) Q^{-1} B y.$$

Substituting z from the above relation and  $x = -A_{11}^{-1}A_{12}y$  in (2.1b), we obtain

$$A_{12}^{T}A_{11}^{-1}A_{12}y + (1-\lambda)\bar{A}_{22}y + \left(1-\lambda(1-\gamma\alpha^{-1})\right)\left(\frac{\lambda-1}{\lambda}\right)\left(\alpha B^{T}Q^{-1}By\right) = 0,$$

having in mind that  $A_{21} = -A_{12}^T$ . For ease of notation we set

$$p := y^* A_{12}^T A_{11}^{-1} A_{12} y, \quad q := y^* \bar{A}_{22} y \text{ and } t := \alpha y^* B^T Q^{-1} B y.$$

Left-multiplying both sides of the preceding relation by  $\lambda y^*$ , we reach to the following quadratic equation:

$$\left(1 + \frac{t}{q}(1 - \gamma\alpha^{-1})\right)\lambda^2 - \left(1 + \frac{t}{q}(1 - \gamma\alpha^{-1}) + \frac{t}{q} + \frac{p}{q}\right)\lambda + \frac{t}{q} = 0$$

$$\lambda^2 - b\lambda + c = 0$$
(2.3)

or, equivalently,

where

$$b := 1 + \frac{p+t}{q+(1-\frac{\gamma}{\alpha})t} \quad \text{and} \quad c := \frac{t}{q+(1-\frac{\gamma}{\alpha})t}.$$
(2.4)

(2.3)

Notice that  $b \ge 1 + c$ . As a result, it is immediate to see that the roots of (2.3) are real and given by

$$\lambda_1 = \frac{b - \sqrt{b^2 - 4c}}{2}$$
 and  $\lambda_2 = \frac{b + \sqrt{b^2 - 4c}}{2}$ .

It is not difficult to see that

$$\begin{aligned} \lambda_{1} &= \frac{2c}{b + \sqrt{b^{2} - 4c}} \\ &\geq \frac{c}{b} = \frac{\alpha y^{*} B^{T} Q^{-1} B y}{y^{*} A_{22} y + p + 2\alpha y^{*} B^{T} Q^{-1} B y} \\ &\geq \frac{\alpha \lambda_{\min}(Q^{-1}) \|By\|_{2}^{2}}{(\lambda_{\max}(A_{22}) + \lambda_{\max}(A_{12}^{T} A_{11}^{-1} A_{12})) + 2\alpha \|B\|_{2}^{2} \lambda_{\max}(Q^{-1})} \\ &\geq \frac{\xi^{2} \alpha \lambda_{\min}(Q)}{\lambda_{\max}(Q)((\lambda_{\max}(A_{22}) + \lambda_{\max}(A_{12}^{T} A_{11}^{-1} A_{12})) \lambda_{\min}(Q) + 2\alpha \|B\|_{2}^{2})} \end{aligned}$$

where  $\xi = \min \{ \|By\|_2 \mid y \notin \text{Ker}(B), y^*y = 1 \}$ . Also, it can be observed that

$$\lambda_{2} \leq b$$

$$= 1 + \frac{p + \alpha y^{*} B^{T} Q^{-1} B y}{y^{*} A_{22} y + \alpha y^{*} B^{T} Q^{-1} B y}$$

$$< 2 + \frac{\lambda_{\max} (A_{12}^{T} A_{11}^{-1} A_{12})}{\lambda_{\min} (A_{22})}.$$
(2.5)



Figure 1: Eigenvalue distributions of  $\bar{\mathcal{A}}$  (top) versus that of the preconditioned matrix  $\mathcal{P}_{\gamma,\alpha}^{-1}\bar{\mathcal{A}}$  (bottom) for different values of  $\gamma$ , with  $Q = \text{diag}(M_p)$  and  $\alpha = 2\gamma$  for a 3D coupled Stokes-Darcy problem with 1695 degrees of freedom.

**Remark 2.1.** As pointed out in [1], for problems of small or moderate size, it can be numerically checked that the condition  $A_{22} > A_{12}^T A_{11}^{-1} A_{12}$  is satisfied for linear systems of the form (1.1) arising from the finite element discretization of coupled Stokes-Darcy flow. Under this condition, for any  $\lambda \in \sigma(\mathcal{P}_{\gamma,\alpha}^{-1}\bar{\mathcal{A}})$  and  $\alpha > 0$ , from Eqs. (2.2) and (2.5), we can deduce that  $0 < \lambda \leq 1 + \tau$  for some  $\tau < 1$ . The previous theorem implies that for fixed n, m and p, as  $\alpha \to \infty$ , except for the possible eigenvalues given by (2.2), any eigenvalue  $\lambda$ (with  $\lambda \neq 1$ ) of the preconditioned matrix tends to 1 as  $\alpha \to \infty$  since in this case the coefficients b and cin Eq. (2.4) go to 2 and 1, respectively. Consequently, the left-hand side of the quadratic equation (2.3) tends to  $(\lambda - 1)^2$  as  $\alpha \to \infty$ . This behavior appears to be confirmed in Fig. 1. While eigenvalues alone do not fully describe the convergence of Krylov subspace methods for nonsymmetric matrices, a well clustered spectrum away from zero is often associated with rapid convergence.

We end this section by some brief comments on the implementation of the proposed preconditioner inside FGMRES. While we do not claim that this implementation is optimal, it gives good results in practice and is competitive with more sophisticated multi-level solvers while having much lower lower set-up costs. To apply the preconditioner, in each inner iteration we need to solve linear systems of the form

$$\mathcal{P}_{\gamma,\alpha}(w_1; w_2; w_3) = (r_1; r_2; r_3).$$

To this end, we use the following block factorization

$$\mathcal{P}_{\gamma,\alpha} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & \gamma B^T Q^{-1} \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} & 0 \\ 0 & A_{22} & B^T \\ 0 & B & -\alpha^{-1} Q \end{bmatrix}$$

which allows one to work with larger values of  $\gamma$ . In fact, we do not have to solve linear systems with

coefficient matrix  $A_{22} + \gamma B^T Q^{-1} B$ . To apply the preconditioner, we need to solve subsystems of the form

$$\begin{bmatrix} A_{22} & B^T \\ B & -\alpha^{-1}Q \end{bmatrix} \begin{bmatrix} w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} r_2 - \gamma B^T Q^{-1} r_3 \\ r_2 \end{bmatrix}.$$
 (2.6)

(note that these systems are of stabilized Stokes type, see [4]). To do so, we use GMRES (with a loose stopping residual tolerance 0.1) in conjunction with the following block triangular preconditioner:

$$P = \begin{bmatrix} \hat{A}_{22} & 0\\ B & -\hat{S} \end{bmatrix}$$

in which  $\hat{A}_{22}$  and  $\hat{S}$  are approximations of  $A_{22}$  and  $S = \alpha^{-1}Q + M_p$  obtained via incomplete Cholesky factorizations constructed by MATLAB function "ichol(., opts)" and MATLAB backslash operator "\", with opts.type ='ict' and opts.droptol = $\epsilon_i$  where  $\epsilon_i$  is respectively equal to  $10^{-3}$  and  $10^{-2}$  for i = 1, 2where  $M_p$  denotes the mass matrix coming from the Stokes pressure space. We further comment that the matrix Q in our numerical implementation is diag $(M_p)$  and  $\alpha = 2\gamma$ , which means that effectively only the parameter  $\gamma$  has to be set by the user. As seen, we also need to solve the linear systems with the coefficient matrix  $A_{11}$  which is solved by PCG with an incomplete Cholesky factorization, as in [1]. The inner PCG iteration was terminated when the relative residual norm was below  $10^{-1}$  or when the maximum number of 5 iterations was reached. These parameter choices, while probably not optimal, were find to be a good compromise in terms of simplicity of implementation, low set-up costs and good preconditioner effectiveness and robustness.

## 3. Numerical experiments

In this section we report on the performance of inexact variants of the proposed block preconditioner using a test problem taken from [3, Subsection 5.3], which corresponds to a 3D coupled flow problem with large jumps in the permeability in the porous flow region. All computations were carried out on a computer with an Intel Core i7-10750H CPU @ 2.60GHz processor and 16.0GB RAM using MATLAB.R2020b.

In Tables 1 and 2 we report the total required number of outer FGMRES iterations and elapsed CPU time (in seconds) under "Iter" and "CPU", respectively. The total number of inner GMRES (PCG) iterations to solve subsystems (2.6) (respectively, with coefficient matrix  $A_{11}$ ) is reported under Iter<sub>in</sub> (Iter<sub>pcg</sub>). No restart is used for either FGMRES or GMRES iterations.

The initial guess is taken to be the zero vector and the iterations are stopped as soon as

$$\|\bar{\mathcal{A}}u_k - \bar{b}\|_2 \leq 10^{-7} \|\bar{b}\|_2$$

where  $u_k$  is the computed k-th approximate solution. In the tables, we also include the relative error

$$\operatorname{Err} := \frac{\|u_k - u^*\|_2}{\|u^*\|_2},$$

where  $u^*$  and  $u_k$  are, respectively, the exact solution and its approximation obtained in the k-th iterate. In addition, we have used right-hand sides corresponding to random solution vectors and averaged results over 10 test runs, rounding the iteration counts to the nearest integer.

The results show that in all cases, the outer FGMRES iteration displays mesh-independent convergence. The number of inner iterations, on the other hand, increases as the mesh is refined, especially for the largest test problem, resulting in less than perfect scalability of the solver. Nevertheless, the total solution time is about 40% less, for the largest problem, than the best results reported in [1], obtained using the multi-level preconditioner ARMS in the solution of the inner subproblems, showing the considerable advantage of the new augmented Lagrangian preconditioner over the original version.

size	$\gamma = 1$				$\gamma = 10$				
	FGMRES		Inner iterations		FGMRES			Inner iterations	
	Iter (CPU)	Err	$Iter_{in}$	$Iter_{pcg}$	Iter (CPU)	Err		$Iter_{in}$	$Iter_{pcg}$
1695	22(0.05)	6.2804 e- 05	128	56	12(0.02)	7.3326e-06		75	33
10809	20(0.52)	1.0262e-04	130	49	12(0.34)	4.1502e-06		88	32
76653	19(4.66)	1.9242e-04	148	58	11(3.02)	2.2011e-05		99	35
576213	19(64.9)	3.8861e-04	248	85	11(38.1)	5.5276e-05		146	45

Table 1: Results for FGMRES in conjunction with preconditioner  $\mathcal{P}_{\gamma,2\gamma}$ .

Table 2: Results for FGMRES in conjunction with preconditioner  $\mathcal{P}_{\gamma,2\gamma}$ .

size	$\gamma = 100$				$\gamma = 1000$				
	FGMRES		Inner iterations		FGMRES		Inner iterations		
	Iter (CPU)	Err	$Iter_{in}$	$\operatorname{Iter}_{pcg}$	Iter (CPU)	Err	$Iter_{in}$	$\operatorname{Iter}_{pcg}$	
1695	11(0.02)	2.6911e-06	63	29	11(0.02)	2.3876e-06	62	28	
10809	11(0.29)	1.1382e-06	71	26	11(0.28)	1.5137e-06	69	25	
76653	11(2.70)	5.1225e-06	86	30	11(2.66)	2.9047 e-06	86	29	
576213	11(36.4)	1.4794 e-05	133	38	11(35.6)	1.3158e-05	130	37	

# 4. Conclusions

In this paper we have introduced a new augmented Lagrangian-based preconditioner for block three-by-three linear systems, with a focus on the linear systems arising from finite element discretizations of the coupled Darcy-Stokes flow problem. The main advantage of this preconditioner is that it avoids the need to explicitly form the augmented block  $A_{22} + \gamma B^T Q^{-1}B$ . Theoretical analysis shows a strong clustering of the spectrum of the (exactly) preconditioned matrix, and numerical experiments on a challenging 3D model problem show that the corresponding inexact preconditioner can result in much faster convergence than previous versions of the augmented Lagrangian-based preconditioner.

Future work will focus on replacing the incomplete Cholesky inner preconditioners with multilevel preconditioners, in order to obtain better scalability of the solver.

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