Parameter robust preconditioning for multi-compartmental Darcy equations

Eleonora Piersanti, Marie E. Rognes, and Kent-Andre Mardal

Abstract In this paper, we propose a new finite element solution approach to the multi-compartmental Darcy equations describing flow and interactions in a porous medium with multiple fluid compartments. We introduce a new numerical formulation and a block-diagonal preconditioner. The robustness with respect to variations in material parameters is demonstrated by theoretical considerations and numerical examples.

1 Introduction

The multi-compartment Darcy equations extend the single compartment Darcy model and describe fluid pressures in a rigid porous medium permeated by multiple interacting fluid networks. These equations have been used to model perfusion in e.g. the heart [8,4], the brain [3] and the liver [1]. The static variant of the equations read as follows: for a given number of networks $J \in \mathbb{N}$, find the network pressures $p_j$ for $j = 1, \ldots, J$ such that

$$- K_j \text{div} \nabla p_j + \sum_{i=1}^{J} \xi_{j-i}(p_j - p_i) = g_j \text{ in } \Omega,$$

\[ (1) \]

1 In this paper, we will also refer to these equations as the multiple–network porosity (MPT) equations.
where $p_j = p_j(x)$ for $x \in \Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$), and $\Omega$ is the physical domain. The scalar parameter $K_j > 0$ represents the permeability of each network $j$. The parameter $\xi_{j-i} \geq 0$ is the exchange coefficient into network $j$ from network $i$. These are assumed to be symmetric: $\xi_{j-i} = \xi_{i-j}$. The right hand side is a source/sink term for each $j$. For simplicity, let $p_j = 0$ on $\partial \Omega$ for $1 \leq j \leq J$.

The system of equations is elliptic as long as $K_j > 0$, but for $K_j \ll \xi_j$ the diagonal dominance is lost for smooth components for which $\|K_j^{1/2} \nabla p_j\| \leq \|\xi_j^{1/2} p_j\|$. As diagonal dominance is often exploited in standard preconditioning algorithms such as for example multigrid, the consequence is a loss of performance. Here, we will therefore propose a transformation of the system of equations that enable the use of standard preconditioners. In detail, we propose and analyze a new approach to constructing finite element formulations and associated block–diagonal preconditioners of the form. The key idea is to change variables through a transformation $T$ that gives simultaneous diagonalization by congruence of the operators involved. We preface and motivate the new approach by a demonstration of lack of robustness of a standard formulation for high exchange parameters.

2 Lack of parameter robustness in standard formulation

A standard variational formulation of (1) reads as follows: find $p_j \in H^1_0 = H^1_0(\Omega)$ for $1 \leq j \leq J$ such that:

\[
(K_j \nabla p_j, \nabla q_j) + \sum_{i=1}^J (\xi_{j-i}(p_j - p_i), q_j) = (g_j, q_j) \quad \forall q_j \in H^1_0,
\]

(2)

where $(\cdot, \cdot)$ denotes the $L^2(\Omega)$ inner product. The system (2) can be written in the alternative form:

\[
k(p, q) + e(p, q) = (g, q),
\]

(3)

with $p = (p_1, p_2, \ldots, p_J)$, $q = (q_1, q_2, \ldots, q_J)$, $g = (g_1, g_2, \ldots, g_J)$, and with matrix form

\[
\mathcal{A}p = g,
\]

where

\[
\mathcal{A} = \mathcal{K} + \mathcal{E} = \begin{pmatrix}
K_1 \Delta & 0 & \cdots & 0 \\
0 & K_2 \Delta & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & K_J \Delta
\end{pmatrix} + \begin{pmatrix}
\sum_{i=1}^J \xi_{1-i} & -\xi_{1-2} & \cdots & -\xi_{1-J} \\
-\xi_{1-2} & \sum_{i=1}^J \xi_{2-i} & \cdots & -\xi_{2-J} \\
\vdots & \vdots & \ddots & \vdots \\
-\xi_{1-J} & -\xi_{2-J} & \cdots & \sum_{i=1}^J \xi_{J-i}
\end{pmatrix}.
\]

Taking the blocks on the diagonal of $\mathcal{A}$ we can immediately define a block diagonal preconditioner $\mathcal{B}$:

\[
\mathcal{B} = \text{diag} \left( -K_1 \Delta + \sum_{i=1}^J \xi_{1-i}, -K_2 \Delta + \sum_{i=1}^J \xi_{2-i}, \cdots, -K_J \Delta + \sum_{i=1}^J \xi_{J-i} \right)
\]

(4)
By definition and by applying the Poincaré inequality, we find that there exists a constant $C_\Omega$ depending on the domain $\Omega$, such that

$$
\langle p, p \rangle = \sum_{i=1}^{J} \sum_{j=1}^{J} (\xi_{j-i}(p_j - p_i), p_j) = \frac{1}{2} \sum_{j=1}^{J} \sum_{i=1}^{J} \xi_{j-i}||p_j - p_i||^2 \geq 0.
$$

By definition and by applying the Poincaré inequality, we find that there exists a constant $C_\Omega$ depending on the domain $\Omega$, such that
\[
(K \mathbf{p}, \mathbf{p}) = \sum_{j=1}^{J} \frac{K_j}{2} \| \nabla p_j \|^2 + \frac{K_j}{2} \| \nabla p_j \|^2 \geq \frac{1}{2} \sum_{j=1}^{J} K_j \| \nabla p_j \|^2 + \frac{C \Omega K_j}{\xi_j} \| p_j \|^2. \tag{8}
\]

Thus, using the definition of \( \mathcal{B} \), we obtain that
\[
(K \mathbf{p}, \mathbf{p}) \geq \frac{1}{2} \min_j \left( 1, \min_j \frac{C \Omega K_j}{\xi_j} \right) (\mathcal{B} \mathbf{p}, \mathbf{p}). \tag{9}
\]

We observe that the coercivity constant depends on the permeability and exchange parameters and is such that it vanishes for vanishing ratios of \( K_j \) to \( \xi_j \).

We can also show that there exists a constant \( \beta \) such that
\[
(\mathcal{A} \mathbf{p}, \mathbf{q}) \leq \beta \| \mathbf{p} \|_{\mathcal{B}} \| \mathbf{q} \|_{\mathcal{B}}. \tag{10}
\]

For any \( \mathbf{p} \) and \( \mathbf{q} \), applying the Cauchy–Schwartz inequality twice we obtain
\[
(\mathcal{A} \mathbf{p}, \mathbf{q}) \leq \sum_{j=1}^{J} K_j \| \nabla p_j \| \| \nabla q_j \| + \sum_{i=1}^{J} \xi_{j-i} \| p_i \| \| q_j \|. \tag{11}
\]

Applying the Cauchy–Schwartz inequality, the diffusion term is bounded as follows
\[
\sum_{j=1}^{J} K_j \| \nabla p_j \| \| \nabla q_j \| \leq \left( \sum_{j=1}^{J} K_j \| \nabla p_j \|^2 \right)^{1/2} \left( \sum_{j=1}^{J} K_j \| \nabla q_j \|^2 \right)^{1/2}. \tag{12}
\]

For the exchange terms, we can use the Cauchy-Schwartz inequality, the symmetry of the exchange coefficients and Chebyshev’s inequality to show that
\[
\sum_{j=1}^{J} \sum_{i=1}^{J} \xi_{j-i} \| p_i \| \| q_j \| \leq J \left( \sum_{j=1}^{J} \xi_j \| p_j \|^2 \right)^{1/2} \left( \sum_{j=1}^{J} \xi_j \| q_j \|^2 \right)^{1/2}, \tag{13}
\]

and similarly for \( \| p_j \| \) in place of \( \| p_i \| \). Thus (10) holds with continuity constant \( \beta \) equal to \( J + 1 \).

The condition number of the preconditioned continuous system can be estimated as the ratio between (10) and (8), c.f. for example [7], and tends to \( \infty \) as \( \xi_{j-i} \to \infty \). CG convergence is governed by the square root of the condition number which in Example[1] explains how the number of iterations increase as \( \xi_{1-2} \) grows in Table[1].

3 Change of variables yields parameter robust formulation

In this section, we present a new approach to variational formulations for the MPT equations. The key idea is to change from variables \( \mathbf{p} \) to variables \( \tilde{\mathbf{p}} \) via a transformation \( T \) such that the equation operators decouple. We can show that this is always possible by simultaneous diagonalization of matrices by congruence.

To this end, we define \( \tilde{\mathbf{p}} \) and \( \tilde{\mathbf{q}} \) as a new set of variables such that
\[
\mathbf{p} = T \tilde{\mathbf{p}}, \quad \mathbf{q} = T \tilde{\mathbf{q}}. \tag{11}
\]
for a linear transformation map (matrix) $T : \mathbb{R}^J \to \mathbb{R}^J$ to be further specified. Substituting (11) into (3), we obtain a new variational formulation reading as: find $\tilde{p} \in (H_0^1)^J$ such that

$$k(T\tilde{p}, T\tilde{q}) + e(T\tilde{p}, T\tilde{q}) = \left(T^T g, \tilde{q}\right) \quad \forall \tilde{q} \in (H_0^1)^J.$$  \hfill (12)

The matrix form of the system is

$$\tilde{A}\tilde{p} = (\tilde{K} + \tilde{E})\tilde{p} = T^T g = \tilde{g},$$  \hfill (13)

where

$$\bar{K} = (-\Delta)\bar{K}, \quad \bar{E} = T^T ET,$$

where the matrix $E \in \mathbb{R}^J \times \mathbb{R}^J$ is given in Section 2 and where we write $K = \text{diag}(K_1, K_2, \ldots, K_J)$.

The key question is now whether there exists an (invertible) transformation $T$ that simultaneously diagonalizes (by congruence) $K$ and $E$? More precisely, is there a matrix $T \in \mathbb{R}^J \times \mathbb{R}^J$ such that

$$\bar{K} = \text{diag}(\bar{K}_1, \bar{K}_2, \ldots, \bar{K}_J), \quad \bar{E} = \text{diag}(\bar{\xi}_1, \bar{\xi}_2, \ldots, \bar{\xi}_J) \ ?$$  \hfill (15)

By matrix analysis theory, see e.g. [2, Theorem 4.5.17, p. 287], there exists indeed such a $T$ since $K$ is diagonal and non-singular and $E$ is symmetric and thus $C = K^{-1}E$ is diagonalizable. In particular, consider the case where $C$ has $J$ distinct eigenvalues $\lambda_j$ and eigenvectors $v_j$ for $j = 1, \ldots, J$. By taking $T = [v_1, v_2, \ldots, v_J]$, (15) holds. Moreover, the eigenvalues $\lambda_j$ are all real.

**Example 2** To exemplify, we here show the diagonalization by congruence of a general 2–network system explicitly. Let

$$K = \begin{pmatrix} K_1 & 0 \\ 0 & K_2 \end{pmatrix}, \quad E = \begin{pmatrix} \xi_{1-2} & -\xi_{1-2} \\ -\xi_{1-2} & \xi_{1-2} \end{pmatrix}.$$  

Then,

$$C = K^{-1}E = \begin{pmatrix} \xi_{1-2}/K_1 & -\xi_{1-2}/K_1 \\ -\xi_{1-2}/K_2 & \xi_{1-2}/K_2 \end{pmatrix},$$

has eigenvalues $e_1 = 0$ and $e_2 = \xi_{1-2}(K_1 + K_2)/(K_1K_2)$ and the eigenvectors form the columns of $T$:

$$T = \begin{pmatrix} 1 & K_2(\xi_{1-2}/K_2 - \xi_{1-2}(K_1 + K_2)/(K_1K_2))/\xi_{1-2} \\ 1 & 1 \end{pmatrix},$$

Finally, we can verify that

$$\bar{K} = T^T KT = \begin{pmatrix} K_1 + K_2 & 0 \\ 0 & K_2(K_1 + K_2)/K_1 \end{pmatrix}.$$
\[ E = T^T ET = \begin{pmatrix} 0 & 0 \\ 0 & \xi_{1-2}(K_1^2 + K_2 + K_2(K_1 + K_2))/K_1^2 \end{pmatrix}. \]

As the transformed system is diagonal and decoupled, a block–diagonal preconditioner is readily available. In particular, we define
\[ \tilde{B} = \tilde{A} = \text{diag}(\tilde{\xi}_1\Delta, \tilde{\xi}_2\Delta, \ldots, \tilde{\xi}_J\Delta) \] (16)
with norm
\[ \|\tilde{p}\|_\tilde{B}^2 = (\tilde{B}\tilde{p}, \tilde{p}) = \sum_{j=1}^J (\tilde{\xi}_j \nabla \tilde{p}_j, \nabla \tilde{p}_j) + \tilde{\xi}_j (\tilde{p}_j, \tilde{p}_j). \] (17)

Clearly, by definition, \( \tilde{A} \) and \( \tilde{B} \) are trivially spectrally equivalent (with upper and lower bounds independent of the material parameters).

4 Numerical examples for the new formulation

In this section, we present numerical results supporting the theoretical considerations. All numerical experiments have been conducted using a finite element discretization, using the FEniCS library [5] and the cbc.block package [6]. To discretize the pressures \( p_j \) and the transformed variables \( \tilde{p}_j \), we consider continuous piecewise linear (\( P_1 \)) finite elements defined relative to each mesh \( \mathcal{T}_h \) of the domain \( \Omega = [0, 1]^2 \). We impose homogeneous Dirichlet conditions on the whole boundary, and zero right hand side(s). The linear systems were solved using a conjugate gradient (CG) solver, with algebraic multigrid (Hypre AMG) with the respective preconditioners, starting from a random initial guess. The tolerance is set to \( 10^{-9} \), iterations are stopped at 3000, the condition number is just an estimation provided by the Krylov spaces involved in the iterations and will be lower than the real value.

Example 3 We first compare the performance of the preconditioners (4) and (16). We let \( K_1 = 1.0 \), and consider different values of the parameters \( K_2, \xi_{1-2} \) and different mesh resolutions \( N \). For the standard formulation (Table 2), the number of iterations (and condition number) is not bounded and increases with the ratio between \( \xi_{1-2} \) and \( K_2 \). We see that the growth is somewhat less than the predicted linear growth. In contrast, for the new formulation (Table 3), we observe that both the number of iterations and the condition number stays nearly constant across the whole range of parameter values tested.

Example 4 In this final example, we study the performance of the preconditioner (16) for three networks. We report the results for \( K_1 = 1.0 \), and different values of the parameters \( K_2, K_3, \xi_{1-2}, \xi_{1-3}, \xi_{2-3} = (10^{-4}, 10^{-2}, 10^0, 10^2, 10^4) \) and different mesh resolutions \( N = (16, 32, 64) \). The results are shown in Figure 1. We observe that the number of iterations stays between 4 and 6 across the whole range of parameters tested, with condition numbers estimated in the range \( 1.0 - 1.25 \).
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| $\xi_{1-2}$ | $K_2$ | $N = 8$ | $N = 16$ | $N = 32$ | $N = 64$ | $N = 128$ |
|------------|-------|--------|--------|--------|--------|--------|
| $10^{-6}$  | 277 (2139) | 1178 (2135) | 2395 (2035) | 3001 (2034) | 3001 (2034) |
| $10^{-4}$  | 280 (2139) | 1180 (2135) | 2283 (2035) | 2860 (2034) | 3001 (2034) |
| $10^{-2}$  | 275 (2117) | 1181 (2113) | 2325 (2014) | 2859 (2013) | 2988 (2011) |
| $10^0$     | 242 (1054) | 935 (1026) | 1629 (1012) | 1556 (1014) | 1557 (1014) |
| $10^2$     | 62 (21) | 74 (22) | 74 (22) | 66 (22) | 64 (22) |
| $10^4$     | 12 (1.6) | 11 (1.6) | 11 (1.6) | 11 (1.6) | 10 (1.6) |
| $10^6$     | 7 (1.1) | 7 (1.1) | 7 (1.1) | 7 (1.1) | 7 (1.1) |
| $10^{-6}$  | 138 (34499) | 692 (42936) | 2999 (45584) | 3001 (17128) | 3001 (5730) |
| $10^{-4}$  | 133 (33287) | 773 (43459) | 2967 (45532) | 3001 (17192) | 3001 (5774) |
| $10^{-2}$  | 141 (36327) | 695 (41605) | 2982 (45144) | 3001 (16773) | 3001 (5657) |
| $10^0$     | 366 (105246) | 1816 (111467) | 3001 (22961) | 3001 (9060) | 3001 (3623) |
| $10^2$     | 280 (2117.4) | 1110 (2113) | 2608 (2114) | 3001 (2131) | 2979 (2111) |
| $10^4$     | 65 (22) | 77 (22) | 74 (22) | 67 (22) | 64 (22) |
| $10^6$     | 12 (1.6) | 12 (1.6) | 11 (1.6) | 11 (1.6) | 10 (1.6) |

Table 2 Number of iterations (and condition number estimates) of a CG solver of the system $\text{feq:mpt:vf}$ with an algebraic multigrid (Hypre AMG) preconditioner of the form (4).

| $\xi_{1-2}$ | $K_2$ | $N = 8$ | $N = 16$ | $N = 32$ | $N = 64$ | $N = 128$ |
|------------|-------|--------|--------|--------|--------|--------|
| $10^{-6}$  | 8 (1.2) | 9 (1.2) | 9 (1.2) | 9 (1.2) | 9 (1.2) |
| $10^{-4}$  | 8 (1.2) | 9 (1.2) | 9 (1.2) | 9 (1.2) | 9 (1.2) |
| $10^{-2}$  | 8 (1.2) | 9 (1.2) | 9 (1.2) | 8 (1.2) | 7 (1.1) |
| $10^0$     | 8 (1.2) | 8 (1.1) | 6 (1.1) | 6 (1.1) | 6 (1.1) |
| $10^2$     | 8 (1.1) | 7 (1.1) | 6 (1.1) | 6 (1.1) | 6 (1.1) |
| $10^4$     | 7 (1.1) | 6 (1.1) | 6 (1.1) | 6 (1.1) | 7 (1.1) |
| $10^6$     | 7 (1.1) | 6 (1.1) | 6 (1.1) | 6 (1.1) | 7 (1.1) |

Table 3 Number of iterations (and condition number estimates) of a CG solver of the system (12) with an algebraic multigrid (Hypre AMG) preconditioner of the form (15).

5 Conclusion

In this paper we have introduced a transformation, based on the congruence of the involved matrices, that transforms MPT systems to a form where diagonal block preconditioners are highly effective. The transformation removes a problem that elliptic
Each point on the graphs represents a simulation performed with different parameters. The color represents the magnitude of $\xi_{1,2} + \xi_{1,3} + \xi_{2,3}$ from smaller (blue) to larger (red). Left: the condition number of the operator versus the number of iterations. Right: condition number versus the ratio between the sum of $\xi_{j,i}$ and sum of $K_j$ (x-axis is logarithmic, y-axis is linear).

systems may have when the elliptic constant is small compared to the continuity constant because of large low order terms.

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