Mixed-Hybrid Formulation of Multidimensional Fracture Flow

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Abstract. We shall study Darcy flow on the heterogeneous system of 3D, 2D, and 1D domains and we present four models for the coupling of the flow. For one of these models, we describe in detail its mixed-hybrid formulation. Finally, we show that Schur complements are suitable for solution of the linear system resulting form the lowest order approximation of the mixed-hybrid formulation.

Keywords: fracture flow, multidimensional coupling, Schur complement

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1 Introduction

The granite rock represents one of the suitable sites for a nuclear waste deposit. Water in the granite massive is conducted by the complex system of fractures of various sizes. While the small fractures can be modeled by an equivalent permeable continuum, the preferential flow in the large geological dislocations and their intersections should be considered as a 2D flow and 1D flow respectively. Motivated by this application, we have developed a simulator (Flow123d) of fracture flow and transport with a multidimensional coupling. Even after several successful applications of this model (e.g. [5]), there is a gap in its theoretical description. The aim of this work is to fill in this gap at least concerning the water flow.

In the second section, we shall present several conceptual models for the coupling between Darcian flows in different dimensions. Then we select one of these models and setup a fully coupled 1-2-3 dimensional problem. In the third section we describe the mixed-hybrid (MH) formulation of the fully coupled problem. We basically follows Maryška, Rozložník, Tůma [6] and Arbogast, Wheeler, Zhang [1], but we rather derive MH-formulation as an abstract saddle point problem in order to use classical theory due to Brezzi and Fortin [2]. Finally, in Section

4 we use Schur complements to solve the linear system resulting from the discretization. We shall prove key properties of the Schur complements similarly as in [7] and we confirm these properties by numerical experiments.

2 Physical Setting

Common model of the underground water flow is the continuity equation

$$\mathrm{div}\boldsymbol{v} = f \tag{1}$$

completed by Darcy's law

$$\boldsymbol{v} = -\mathbb{K}\nabla h, \tag{2}$$

where $\boldsymbol{v}$ is the Darcy flux $[ms^{-1}]$, h is the water pressure head $[m]$, f is the volume density of the water sources $[s^{-1}]$, and $\mathbb{K}$ is the tensor of hydraulic conductivity $[ms^{-1}]$. Let us consider the water flow described by (1), (2) in a 3D porous medium that contains very thin layers and channels with a substantially different hydraulic conductivity. Due to the different conductivity these features can not be neglected, but can be considered as 2D and 1D objects respectively. We denote $\Omega_3 \subset \mathbf{R}^3$ the 3D domain, $\Omega_2 \subset \Omega_3$ will be the domain of 2D fractures, and $\Omega_1 \subset \Omega_2$ is the domain of 1D channels. In order to keep further formulas consistent, we also introduce Ω_0 as the set of channel intersections. Since the fractures and channels are thin, we can assume that the velocity and the pressure is constant in the normal direction. Moreover the normal part of the velocity can be interpreted as the water interchange with the surrounding medium. Consequently we can integrate (1) along the normal directions and obtain

$$\mathrm{div}\boldsymbol{q}_d = F_d \quad \text{on } \Omega_d \setminus \Omega_{d-1} \quad \text{for } d \in \{1,2,3\}, \tag{3}$$

where $\boldsymbol{q}_3 = \boldsymbol{v}_3$ is simply the Darcy flux $[ms^{-1}]$, $\boldsymbol{q}_2 = \delta_2\boldsymbol{v}_2$ $[m^2s^{-1}]$ is the water flux through the 2D fracture of thickness δ_2 $[m]$, and $\boldsymbol{q}_1 = \delta_1\boldsymbol{v}_1$ $[m^3s^{-1}]$ is the water flux through the 1D channel of cross-section δ_2 $[m^2]$. Further, F_d are partially integrated densities of the water sources, which we shall discuss presently. Vectors $\boldsymbol{q}_d$ and tensors $\mathbb{K}_d$, $d \in \{1,2,3\}$ lives in the corresponding tangent space of Ω_d. Similarly, we denote h_d the pressure head on the domain Ω_d.

Next, we have to introduce suitable coupling between the equations on the domains of different dimension. We assume that the water flux q_{ab} from Ω_a to Ω_b is driven by the pressure head difference:

$$q_{ab} = \sigma_{ab}(h_a - h_b), \tag{4}$$

where σ_{ab} is an water transition coefficient. However, there are at least four different models for 2D-1D and 3D-2D interaction based on the equation (4).

Let us explain it on 2D-1D case (see Figure 2). We can choose either discontinuous or continuous pressure head on 2D. In the first case there is one independent water interchange for each of two sides of the 1D domain and the 2D pressure head is discontinuous over the 1D fracture. Thats why we call it

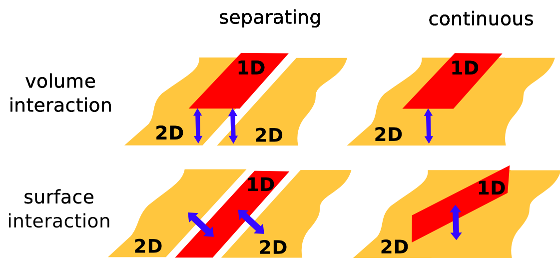

Fig. 1. Four possible interaction models between 2D and 1D.

also a *separating fracture*. In the second case we assume continuous 2D pressure and only one total flux between 2D and 1D.

Independently, we can choose either communication over the volume or over the surface. In the case of the volume communication the flux q_{ab} acts as a volume source $[s^{-1}]$ in both dimension. Nevertheless, to keep it constant in the normal direction of the 1D domain, we have to perform averaging of q_{ab} over the width δ $[m]$ of the 1D domain. The transition coefficient σ has unit $[m^{-1}s^{-1}]$ and has the same meaning as the water transfer coefficient in the dual continuum models (see [3]). In the case of the surface communication, the outflow q_{ab} $[ms^{-1}]$ from the boundary of the 2D domain spreads over the width δ $[m]$ of the 1D domain so that q_{ab}/δ act as a volume source in the 1D domain. The transition coefficient σ $[s^{-1}]$ should be proportional to $|\mathbb{K}|\delta$.

In what follows, we consider only the model with discontinuous pressure head and the surface communication. On the domain Ω_2, there is one water outflow from Ω_3 for every side of the surface:

$$\boldsymbol{q}_3 \cdot \boldsymbol{n}^+ = q_{32}^+ = \sigma_3^+(h_3^+ - h_2),$$
$$\boldsymbol{q}_3 \cdot \boldsymbol{n}^- = q_{32}^- = \sigma_3^-(h_3^- - h_2),$$

where $\boldsymbol{q}_3 \cdot \boldsymbol{n}^{+/-}$ $[ms^{-1}]$ is the outflow from Ω_3, $h_3^{+/-}$ $[m]$ is the trace of the pressure head on Ω_3, h_2 $[m]$ is the pressure head on Ω_2, and $\sigma_3^{+/-} = \sigma_{32}$ $[s^{-1}]$ is the transition coefficient. On the other hand, the sum of the interchange fluxes $\boldsymbol{q}_{32}^{+/-}$ forms a volume source on Ω_2. Therefore F_2 $[ms^{-1}]$ on the right hand side of (3) is given by

$$F_2 = \delta_2 f_2 + (q_{32}^+ + q_{32}^-). \tag{5}$$

The communication between Ω_2 and Ω_1 is similar. However, in the 3D ambient space, an 1D channel can adjoining multiple 2D fractures $1, \dots, n$. Therefore, we have n independent outflows from Ω_2:

$$\boldsymbol{q}_2 \cdot \boldsymbol{n}^i = q_{21}^i = \sigma_2^i(h_2^i - h_1),$$

where $\sigma_2^i = \delta_2^i \sigma_{21}$ $[ms^{-1}]$ is the transition coefficient integrated over the width of the fracture i. Sum of the fluxes forms F_1 $[m^2 s^{-1}]$

$$F_1 = \delta_1 f_1 + \sum_i q_{21}^i. \tag{6}$$

For the consistency we also set $F_3 = f_3$ $[s^{-1}]$, $\delta_3 = 1$ $[-]$, and $\sigma_1 = 0$.

In order to obtain unique solution we have to prescribe boundary conditions. We assume that $\partial\Omega_1 \subset \partial\Omega_2 \subset \partial\Omega_3$. Let us denote Γ_d^D the Dirichlet part of the boundary $\partial\Omega_d$, where we prescribe the pressure head P_d. On the remaining part Γ_d^W, we prescribe outflow by the Newton boundary condition

$$\boldsymbol{q}_d \cdot \boldsymbol{n} = \alpha_d (h_d - P_d^W).$$

where α_3 $[s^{-1}]$, α_2 $[ms^{-1}]$, α_1 $[m^2 s^{-1}]$ are a transition coefficients and P_d^W is the given outer pressure head.

3 Mixed-Hybrid Formulation of Multidimensional Fracture Flow Problem

Now, we are going to introduce MH-formulation of the problem denoted in the previous section. To avoid technicalities, we assume that Ω_3 have piecewise polygonal boundary, domain Ω_2 consists of polygons, and Ω_1 consists of line segments. We also assume $\partial\Omega_1 \subset \partial\Omega_2 \subset \partial\Omega_3$. Further, we decompose Ω_d, $d \in \{1, 2, 3\}$ into sub-domains Ω_d^i, $i \in I_d$ satisfying the compatibility condition

$$\Omega_{d-1} \subset \Gamma_d \setminus \partial\Omega_d, \quad d = 1, 2, 3 \quad \text{where } \Gamma_d = \bigcup_{i \in I_d} \partial\Omega_d^i. \tag{7}$$

The idea of MH-formulation is to integrate (2) by parts on every sub-domain. There appears a term with the trace of the pressure head, which is considered as a Lagrange multiplier to enforce continuity of the pressure head over the boundaries. However, since the pressure head could be discontinuous over the fractures, we have to deal with two distinct multipliers along Ω_2 and Ω_1. To this end, we introduce a natural decomposition Ω_d^j, $j \in J_d$ with boundaries given by Ω_{d-1}. Due to the compatibility condition (7) the decomposition I_d can be viewed as a refinement of the decomposition J_d. In particular, for every Ω_d^i, $i \in I_d$ there is a unique $j(i)$ such that $\Omega_d^i \subset \Omega_d^{j(i)}$. Then the Lagrange multiplier for the sub-domain Ω_d^j, $j \in J_d$ have support on the set

$$\Gamma_d^j = \Gamma_d \cap \overline{\Omega_d^j}. \tag{8}$$

Following [1] and [6], we shall consider following spaces for the MH-solution:

$$V = V_3 \times V_2 \times V_1 = \prod_{d \in 3,2,1} \prod_{i \in I_d} H(\mathrm{div}, \Omega_d^i), \tag{9}$$

$$P = P_3 \times P_2 \times P_1 \times \mathring{P}_3 \times \mathring{P}_2 \times \mathring{P}_1, \tag{10}$$

$$P_d = L^2(\Omega_d), \quad \mathring{P}_d = \prod_{j \in J_d} \left\{ \mathring{\varphi} \in H^{1/2}(\Gamma_d^j) \,|\, \mathring{\varphi} = 0 \text{ on } \Gamma_d^D \right\}.$$

where $H(\mathrm{div}, \Omega)$ is standard space of L^2-vector functions with divergence in $L^2(\Omega)$, and $H^{1/2}(\partial\Omega)$ is the space of traces of functions from $H^1(\Omega)$. In the definition of the MH-solution, the flux $\boldsymbol{q}_d$ is from V_d, the pressure head h_d from P_d and the Lagrange multiplier or the pressure head trace $\mathring{h}$ is from $\mathring{P}_d$. Introduction of the composed spaces V and P allows us to formulate MH-problem as an abstract saddle problem in the spirit of [2]

Definition 1. *We say that pair $(\boldsymbol{q}, h) \in V \times P$ is MH-solution of the problem if it satisfy abstract saddle point problem*

$$a(\boldsymbol{q}, \boldsymbol{\psi}) + b(\boldsymbol{\psi}, h) = \langle F, \boldsymbol{\psi}\rangle \qquad \forall \boldsymbol{\psi} \in V, \tag{11}$$

$$b(\boldsymbol{q}, \varphi) - c(h, \varphi) = \langle G, q\rangle \qquad \forall \varphi \in P, \tag{12}$$

where bilinear forms on the left-hand side are

$$a(\boldsymbol{q}, \boldsymbol{\psi}) = \sum_{d=1,2,3}\sum_{i\in I_d}\int_{\Omega_d^i} \frac{1}{\delta_d}\boldsymbol{q}_d^i \mathbb{K}_d^{-1}\boldsymbol{\psi}_d^i,$$

$$b(\boldsymbol{q}, \varphi) = \sum_{d=1,2,3}\sum_{i\in I_d}\left(\int_{\Omega_d^i} -\mathrm{div}\boldsymbol{q}_d^i\varphi_d + \int_{\partial\Omega_d^i}(\boldsymbol{q}_d^i\cdot\boldsymbol{n})\mathring{\varphi}_d^{j(i)}\right),$$

$$c(h, \varphi) = \sum_{d=1,2,3}\sum_{j\in J_d}\left(\int_{\Gamma_d^j\cap\Omega_{d-1}} \sigma_d(h_{d-1} - \mathring{h}_d^j)(\varphi_{d-1} - \mathring{\varphi}_d^j) + \int_{\Gamma_d^j\cap\Gamma_d^W}\alpha_d\mathring{h}_d^j\mathring{\varphi}_d^j\right),$$

and linear forms on the right-hand side are

$$\langle G, \boldsymbol{\psi}\rangle = \sum_{d=1,2,3}\sum_{i\in I_d}\int_{\partial\Omega_d^i}\tilde{P}_d(\boldsymbol{\psi}_d\cdot\boldsymbol{n}),$$

$$\langle F, \varphi\rangle = -\sum_{d=1,2,3}\left(\int_{\Omega_d}\delta_d f_d\varphi_d + \sum_{j\in J_d}\int_{\Gamma_d^j\cap\Gamma_d^W}\alpha_d P_d^W\mathring{\varphi}_d^j\right).$$

where $\tilde{P}_d \in \mathring{P}_d$ is any extension of the Dirichlet condition $P_d \in H^{1/2}(\Gamma_d^D)$. Consequently the full trace of the unknown pressure head is $\mathring{h}_d + \tilde{P}_d$.

The second term of the form b deserves a note. The outflow $\boldsymbol{q}_d^i\cdot\boldsymbol{n}$ is from dual to $H^{1/2}(\partial\Omega_d^i)$ which in general is not subspace of $H^{1/2}$ on the larger domain, namely $\Gamma_d^{j(i)}$. But here we use the fact, that the later domain does not penetrate into the domain Ω_d^i.

Assuming that δ_d, $\mathbb{K}_d$, σ_d, and α_d are uniformly bounded and uniformly grater then zero (positive definiteness of $\mathbb{K}_d$), we can prove that $a(\cdot,\cdot)$ and $c(\cdot,\cdot)$ are bounded, symmetric, positive definite bilinear forms and that

$$\mathcal{B} : V \to P', \quad \langle\mathcal{B}(\boldsymbol{q}, \varphi\rangle = b(\boldsymbol{q}, \varphi)$$

is surjective operator. Assuming further

$$f_d \in L^2(\Omega_d),\ P_d \in H^{1/2}(\Gamma_d^D),\ P_d^W \in L^2(\Gamma_d^W),$$

we can prove that the MH-solution is independent of choice of decomposition I_d and independent of choice of extension $\tilde{P}_d$. Finally, using [2, Theorem 1.2], we can prove existence and uniqueness of the MH-solution.

4 Linear System and Its Schur Complements

Advantage of the discretizations based on mixed-hybrid formulation is a particular form of the resulting linear system, which could be effectively solved by Schur complements. In this section, we shall investigate Schur complements in the case of our coupled problem.

We consider the lowest order approximation of the MH-formulation. To this end, we choose simplexes as the sub-domains Ω_d^i, $i \in I_d$. Then, we approximate the space $H(\mathrm{div}, \Omega_d^i)$ by the Raviart-Thomas space $RT_0(\Omega_d^i)$ (see [2]) and the spaces $L^2(\Omega_d)$ and $H^{1/2}(\Gamma_d^j)$ by piecewise constant functions on elements and their edges respectively (for details see [6]). Such discretization leads to the linear system which inherits the saddle-point structure of the system (11), (12). The whole matrix $\mathbb{A}$ has a form

$$\mathbb{A} = \begin{pmatrix} A & B^T & \mathring{B}^T \\ B & C & \mathring{C}^T \\ \mathring{B} & \mathring{C} & \tilde{C} \end{pmatrix}$$

where block A is discrete version of $a(\,\cdot\,,\,\cdot\,)$ and consists of positive-definite blocks $(d+1) \times (d+1)$ on the diagonal. Therefore, the inverse A^{-1} is also positive-definite and easy to compute. The rows and columns of A correspond to all sides of elements of the mesh. The blocks B and $\mathring{B}$ come from the first and the second term of the form $b(\,\cdot\,,\,\cdot\,)$ respectively. Rows of B correspond to elements, rows of $\mathring{B}$ correspond to the neighbourings of sides. The block B has $(d+1)$ non-zeroes at the row of a d-dimensional element located in the columns of its sides. The block $\mathring{B}$ has one non-zero value per column (side) with value 1. The blocks C, $\mathring{C}$, $\tilde{C}$ are discretizations of the form $-c(\,\cdot\,,\,\cdot\,)$, thus whole C-block is negative-definite. In Figure 4 (a), you can see the matrix $\mathbb{A}$ for a testing problem P1 — a cube cut by two diagonal planes (fractures) into four prisms. Notice the four semi-triangular shapes in the block $\mathring{B}$, which are formed by the internal neighbourings of the elements inside of the prisms.

Full analysis of the system matrix and its Schur complements for a 3D domain and prismatic finite elements was done by Maryška, Rozložník, and Tůma in [7]. Here we only mention main properties. As A^{-1} is positive-definite and C is negative-definite, the first Schur complement

$$\mathbb{A}/A = C - (B\,\mathring{B})^T A^{-1} (B\,\mathring{B})$$

is negative-definite. Moreover, $\mathbb{A}_1 = B^T A^{-1} B$ is diagonal. Hence we can perform the second Schur complement $\mathbb{A}_2 = (-\mathbb{A}/A)/\mathbb{A}_1$. (see Figure 4 (b), (c)).

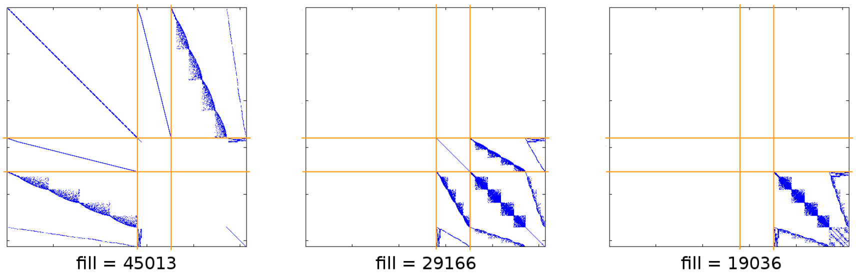

Fig. 2. Sparsity pattern: (a) original matrix (b) first Schur complement (c) second Schur complement

We shall prove that $\mathbb{A}_2$ is positive-definite by showing that the Schur complement of any positive definite matrix is also positive definite. Let

$$M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$$

be positive definite. One can check that

$$M^{-1} = \begin{pmatrix} \overline{A} & \overline{B} \\ \overline{B}^T & \overline{C} \end{pmatrix}$$

where

$$\overline{C} = (M/A)^{-1}, \quad \overline{B} = -A^{-1}B\overline{C}, \quad \overline{A} = A^{-1} + A^{-1}B\overline{B}^T.$$

In particular M/A^{-1} is principal sub-matrix of M^{-1}. Now we use the interlacing property:

Proposition 1. *[4, Theorem 8.1.7] Let $B \in \mathbf{R}^{k \times k}$ be symmetric principal sub-matrix of a symmetric matrix $A \in \mathbf{R}^{n \times n}$. Denoting α_i and β_i decreasing eigenvalues sequence of A and B respectively, it holds*

$$\alpha_i \geq \beta_i \geq \alpha_{i+n-k}, \qquad i = 1, \ldots, k.$$

Consequently the least eigenvalue of M/A is bounded from below by the least eigenvalue of M.

Apart from being positive-definite the Schur complements offer substantial reduction of the problem size. In Table 1, we compare matrices $\mathbb{A}$, $\mathbb{A}1$, $\mathbb{A}_2$ for the problem P1 discretized by 1444 elements. For the second Schur complement, we get reduction of the size by factor 3 and reduction of the fill by factor 2. At the same time, we get also reduction of the condition number.

Table 2 reports results of numerical experiments for problem P1 solved on two different meshes. In all cases we have used BiCGStab method preconditioned by ILU(k) with a factor level k. For every linear system, we were looking for the

Table 1. Comparison of Schur complements.

Schur complement	size	fill	condition number
$\mathbb{A}$	10258	45013	9.8e+05
$\mathbb{A}_1$	4662	29166	1.0e+06
$\mathbb{A}_2$	3218	19036	1.1e+05

factor level k that gives the optimal time of the whole solver. Indeed, for higher factor levels, we get better preconditioning and thus smaller iteration number, but because of the higher fill of the preconditioner, the iterations are slower. An important observation is that in contrast to the whole matrix $\mathbb{A}$, the optimal factor level for the Schur complements is independent of the problem size.

Table 2. Convergence of BiCGStab with ILU and optimal factor level.

	112 755 elements			290 281 elements		
Schur complement	$\mathbb{A}$	$\mathbb{A}_1$	$\mathbb{A}_2$	$\mathbb{A}$	$\mathbb{A}_1$	$\mathbb{A}_2$
ILU factor level	**9**	3	2	**13**	3	3
iterations	45	31	44	42	46	49
solver time	40.4 s	18.6 s	15.4 s	118 s	72 s	63 s

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