Mixed Finite Element Methods for Modeling Flow and Transport in Porous Media

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MIXED FINITE ELEMENT METHODS FOR MODELING FLOW AND TRANSPORT IN POROUS MEDIA*

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Abstract. Mixed finite element methods applied to modeling flow and transport in porous media are discussed for both single and multiphase problems. An expanded mixed finite element method is introduced to treat general geometry problems and full tensor permeability and/or dispersion. Extensions to discontinuous coefficients, multiblock domains, and non-matching grids or faults are also discussed. Convergence results for some of these procedures are presented.

1. Introduction. In this paper, we present a brief summary of results on applying mixed finite element methods for modeling flow and transport in porous media, which have been obtained by several members of the Center for Subsurface Modeling at the University of Texas (formerly the Subsurface Modeling Group at Rice University).

In modeling flow in porous media it is important to employ a discretization method that is accurate, conserves mass locally and preserves continuity of fluxes, i.e. the physics of the problem is satisfied. In addition, the algorithm needs to be able to handle tensor permeabilities and dispersivities and irregularly shaped domains. Finally it is advantageous to be able to implement the procedure as a cell-centered finite difference method and be able to incorporate it into existing petroleum reservoir simulators using rectangular grids or multiblocks.

Here we describe mixed finite element algorithms which satisfy all the above properties. These methods conserve mass locally. For Darcy flow both the pressure and the velocity are approximated with the same order of convergence. Moreover, the flux is forced to be continuous.

We have included in the bibliography a collection of references in which mixed methods have been formulated, analyzed, and/or applied to flow in porous media problems. This list is by no mean comprehensive because of page limitations. We have however referenced the seminal work of Raviart, Thomas, Arnold, Brezzi, Douglas, Roberts and others in the formulation and analysis of mixed methods for elliptic partial differential equations [47, 44, 7, 29] .

Mixed finite element methods have been used in modeling flow in porous media for many years. In the case of miscible displacement in porous media, Douglas, Ewing and Wheeler [27, 28] introduced mixed finite element methods for solving the Darcy flow equation. Further analysis and implementation of these algorithms can be found in [25, 33, 34, 46, 15, 26]. We wish to note however that mixed finite element methods with special numerical quadrature have been employed in petroleum reservoir engineering for more than forty years [43, 8]. This relationship between cell-centered finite differences and mixed finite element methods was first observed and analyzed by Russell and Wheeler in [45]. Superconvergence results were later obtained by Weiser and Wheeler [48]. Other convergence and superconvergence results for the mixed methods can be found in [41, 30, 32]. We note that all of the above works treat diagonal tensor coefficients.

The rest of this paper is divided into three major sections. In Section 2 we discuss

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mixed finite element methods for single phase flow. First, the expanded mixed finite element method [49, 38, 16, 4] is formulated to treat general geometry problems and full tensor permeability or dispersion. In addition special quadratures are introduced to obtain a cell-centered finite difference procedure for treating logically rectangular grids. Extensions to discontinuous coefficients, multiblock domains, and non-matching grids or faults are also discussed. Convergence results for some of these procedures are presented. Also in this section it is noted that the characteristics-mixed method developed by Arbogast and Wheeler [3] for transport or advection-diffusion/dispersion problems is locally conservative.

In Section 3 mixed finite element methods for multiphase flow are considered. Here we show that the standard finite difference procedure used by the petroleum reservoir engineers is an expanded mixed finite element method with special quadrature. In addition mixed methods based on the fractional flow formulation are described.

Some conclusions and current research are provided in the last section of the paper.

2. Mixed finite elements for single phase flow. Flow of a single fluid in porous media is modeled by a second order elliptic equation. Given domain $\Omega \subset \mathbf{R}^d$, $d = 2$ or 3, the problem in its mixed form is to find the velocity $\mathbf{u}$ and the pressure p such that

$$\mathbf{u} = -K\nabla p \qquad \text{in } \Omega, \tag{2.1}$$

$$\nabla \cdot \mathbf{u} = f \qquad \text{in } \Omega, \tag{2.2}$$

$$p = g^D \qquad \text{on } \Gamma^D, \tag{2.3}$$

$$\mathbf{u} \cdot \nu = g^N \qquad \text{on } \Gamma^N. \tag{2.4}$$

Here K is a symmetric positive definite tensor with $L^\infty(\Omega)$ components, representing the permeability divided by the viscosity, and ν is the outward unit normal vector on the boundary $\partial\Omega$, which is decomposed into Γ^D and Γ^N. Equation (2.1) is referred to as Darcy law, and (2.2) is the mass conservation equation.

2.1. The expanded mixed method on general geometry. Two features of the differential problem impose difficulties on its numerical approximation by mixed finite element methods. First, the permeability K is a full tensor, and second, the domain Ω can have irregular geometry. The expanded mixed method has been introduced to handle efficiently these two problems.

Let $(\cdot,\cdot)_S, S \subset \mathbf{R}^d$, denote the $L^2(S)$ inner product or duality pairing. The $L^2(S)$ norm is given by

$$\|\phi\|_{0,S} = (\phi,\phi)_S.$$

The subscript S will be omitted if $S = \Omega$. Let $\langle\cdot,\cdot\rangle_{\partial S}$ denote the $L^2(\partial S)$ inner product or duality pairing. Define

$$H(\mathrm{div}; S) = \{\mathbf{v} \in (L^2(S))^d : \nabla \cdot \mathbf{v} \in L^2(S)\},$$

with the norm

$$\|\mathbf{v}\|_{H(\mathrm{div};S)} = \left\{ \int_S \left(|\mathbf{v}|^2 + |\nabla \cdot \mathbf{v}|^2 \right) dx \right\}^{1/2}.$$

Following [4, 1] we introduce the adjusted pressure gradient

$$\tilde{\mathbf{u}} = -M^{-1}\nabla p,$$

where M is some symmetric positive definite tensor related to the geometry of Ω. Then

$$\mathbf{u} = KM\tilde{\mathbf{u}},$$

and we have the following expanded mixed formulation.

$$(M\mathbf{u}, \tilde{\mathbf{v}}) = (MKM\tilde{\mathbf{u}}, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in (L^2(\Omega))^d, \tag{2.5}$$

$$(M\tilde{\mathbf{u}}, \mathbf{v}) - (p, \nabla \cdot \mathbf{v}) \tag{2.6}$$

$$= -\langle g^D, \mathbf{v} \cdot \nu \rangle_{\Gamma^D} - \langle \lambda, \mathbf{v} \cdot \nu \rangle_{\Gamma^N}, \qquad \mathbf{v} \in H(\mathrm{div}; \Omega),$$

$$(\nabla \cdot \mathbf{u}, w) = (f, w), \qquad w \in L^2(\Omega), \tag{2.7}$$

$$\langle \mathbf{u} \cdot \nu, \mu \rangle_{\Gamma^N} = \langle g^N, \mu \rangle_{\Gamma^N}, \qquad \mu \in H^{1/2}(\Gamma^N), \tag{2.8}$$

where λ is the boundary pressure on Γ^N.

Let $\{\mathcal{T}_h\}_{h>0}$ be a regular family of finite element partitions of Ω [18]. There are many known mixed finite element spaces $\mathbf{V}_h \times W_h \subset H(\mathrm{div}; \Omega) \times L^2(\Omega)$ associated with $\mathcal{T}_h$, in the case of standard shape elements (triangle, tetrahedra, parallelepiped, or prism) [47, 44, 42, 13, 11, 12, 17]. Here we generalize these spaces to curved elements in the following way. Let

$$F : \mathbf{R}^d \to \mathbf{R}^d, \quad F(\hat{\Omega}) = \Omega,$$

be a smooth (at least C^2) invertible map, where $\hat{\Omega}$ is a computational reference domain with a regular shape. Given a partition $\hat{\mathcal{T}}_h$ of $\hat{\Omega}$, F defines a curved element partition $\mathcal{T}_h$ of Ω. Denote by $\hat{\mathbf{V}}_h \times \hat{W}_h$ any of the known mixed spaces defined on $\hat{\mathcal{T}}_h$. Then the spaces $\mathbf{V}_h \times W_h$ are defined in the usual way by the standard isomorphism for the scalar space and the Piola transformation for the vector space. For any scalar function $\hat{\varphi}(\hat{\mathbf{x}})$ on $\hat{\Omega}$, let

$$\varphi(\mathbf{x}) = \hat{\varphi} \circ F^{-1}(\mathbf{x}), \tag{2.9}$$

and for any function $\hat{\mathbf{q}} \in (L^2(\hat{\Omega}))^d$, define

$$\mathbf{q}(\mathbf{x}) = \left(\frac{1}{J} DF\, \hat{\mathbf{q}} \right) \circ F^{-1}(\mathbf{x}), \tag{2.10}$$

where $DF(\hat{\mathbf{x}})$ is the Jacobian matrix of F and

$$J(\hat{\mathbf{x}}) = |\det(DF(\hat{\mathbf{x}}))|.$$

We note that the Piola transformation preserves the normal components of the vectors, therefore the velocity space $\mathbf{V}_h$ is a subspace of $H(\mathrm{div}; \Omega)$.

Let $\Lambda_h^N \subset L^2(\Gamma^N)$ be the corresponding Lagrange multiplier space for the pressure on Γ^N [7, 14]. Let $\tilde{\mathbf{V}}_h$ be a finite element subspace of $(L^2(\Omega))^d$ such that $\mathbf{V}_h \subseteq \tilde{\mathbf{V}}_h$.

In the expanded mixed method on general geometry we solve for $\mathbf{u}_h \in \mathbf{V}_h$, $\tilde{\mathbf{u}}_h \in \tilde{\mathbf{V}}_h$, $p_h \in W_h$, and $\lambda_h \in \Lambda_h^N$ satisfying

$$(M\mathbf{u}_h, \tilde{\mathbf{v}}) = (MKM\tilde{\mathbf{u}}_h, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_h, \tag{2.11}$$

$$(M\tilde{\mathbf{u}}_h, \mathbf{v}) - (p_h, \nabla \cdot \mathbf{v}) \tag{2.12}$$

$$= -\langle g^D, \mathbf{v} \cdot \nu \rangle_{\Gamma^D} - \langle \lambda_h, \mathbf{v} \cdot \nu \rangle_{\Gamma^N}, \qquad \mathbf{v} \in \mathbf{V}_h,$$

$$(\nabla \cdot \mathbf{u}_h, w) = (f, w), \qquad w \in W_h, \tag{2.13}$$

$$\langle \mathbf{u}_h \cdot \nu, \mu \rangle_{\Gamma^N} = \langle g^N, \mu \rangle_{\Gamma^N}, \qquad \mu \in \Lambda_h^N. \tag{2.14}$$

Optimal convergence for $\|p - p_h\|_0$, $\|\lambda - \lambda_h\|_{-1/2}$, $\|\mathbf{u} - \mathbf{u}_h\|_0$, $\|\tilde{\mathbf{u}} - \tilde{\mathbf{u}}_h\|_0$, and $\|\nabla \cdot (\mathbf{u} - \mathbf{u}_h)\|_0$ in all known mixed spaces has been shown in [4, 1] under the assumption of smoothness of K and M. Here we present the results for the lowest order Raviart- Thomas spaces [44, 42].

THEOREM 2.1. *For the expanded mixed method* (2.11)–(2.14) *on curved elements, there exists a constant C, independent of h and dependent on*

$$\hat{\Omega}, \|p\|_2, \|u\|_1, \|\nabla \cdot u\|_1, \|M\|_{1,\infty}, \|K\|_{1,\infty}, \|K^{-1}\|_{0,\infty}, \|F\|_{2,\infty}, \text{ and } \|F^{-1}\|_{2,\infty},$$

such that

$$\|\mathbf{u} - \mathbf{u}_h\|_0 + \|\tilde{\mathbf{u}} - \tilde{\mathbf{u}}_h\|_0 \le Ch, \tag{2.15}$$

$$\|\nabla \cdot (\mathbf{u} - \mathbf{u}_h)\|_0 \le Ch, \tag{2.16}$$

$$\|\mathcal{P}_h p - p_h\|_0 \le Ch^2, \tag{2.17}$$

$$\|p - p_h\|_0 \le Ch, \tag{2.18}$$

$$\|\lambda - \lambda_h\|_{-1/2} \le Ch^{3/2}. \tag{2.19}$$

Here $\|\cdot\|_{j,q,S}$ is the norm of the Sobolev space $W^{j,q}(S)$ of j-times differentiable functions in $L^q(S)$, and $\mathcal{P}_h$ denotes the $L^2(\Omega)$-projection operator onto W_h defined for any $\psi \in L^2(\Omega)$ by

$$(\psi - \mathcal{P}_h\psi, w) = 0, \quad w \in W_h.$$

Note that estimate (2.17) implies superconvergence for $\|\mathcal{P}_h p - p_h\|_0$.

2.2. A Cell-centered finite difference scheme on logically rectangular grids. The main advantage of the expanded mixed formulation is that it can be implemented as cell-centered finite differences for the pressure, even for problems with full tensor coefficients on general geometry domains. In [4], for the case of RT_0 spaces on rectangular grids, quadrature rules are used to approximate some of the integrals. Thus the vector unknowns can be eliminated resulting in a sparse positive definite system for the pressures. Moreover, superconvergence for both pressure and velocity is obtained at certain discrete points. These results have been generalized in [1] to logically rectangular and triangular grids. Special choice of M simplifies the interactions of the vector basis functions in (2.11) and (2.12). Define

$$M(F(\hat{\mathbf{x}})) = \left(J(DF^{-1})^T DF^{-1}\right)(\hat{\mathbf{x}}). \tag{2.20}$$

Using (2.9) and (2.10), problem (2.11)–(2.14) can be transformed into the following problem on the reference domain $\hat\Omega$. Find $\hat{\mathbf{u}}_h \in \hat{\mathbf{V}}_h$, $\hat{\tilde{\mathbf{u}}}_h \in \hat{\tilde{\mathbf{V}}}_h$, $\hat p_h \in \hat W_h$, and $\hat\lambda_h \in \hat\Lambda_h^N$ such that

$$(\hat{\mathbf{u}}_h, \hat{\tilde{\mathbf{v}}})_{\hat\Omega} = \left(JDF^{-1}K(DF^{-1})^T\hat{\tilde{\mathbf{u}}}_h, \hat{\tilde{\mathbf{v}}}\right)_{\hat\Omega}, \qquad \hat{\tilde{\mathbf{v}}} \in \hat{\tilde{\mathbf{V}}}_h, \tag{2.21}$$

$$\begin{aligned}(\hat{\tilde{\mathbf{u}}}_h, \hat{\mathbf{v}})_{\hat\Omega} - (\hat p_h, \hat\nabla\cdot\hat{\mathbf{v}})_{\hat\Omega} & \qquad\qquad (2.22)\\ = -\langle \hat g^D, \hat{\mathbf{v}}\cdot\hat\nu\rangle_{\hat\Gamma^D} - \langle\hat\lambda_h, \hat{\mathbf{v}}\cdot\hat\nu\rangle_{\hat\Gamma^N}, &\qquad \hat{\mathbf{v}} \in \hat{\mathbf{V}}_h,\end{aligned}$$

$$(\hat\nabla\cdot\hat{\mathbf{u}}_h, \hat w)_{\hat\Omega} = (J\hat f, \hat w)_{\hat\Omega}, \qquad \hat w \in \hat W_h, \tag{2.23}$$

$$\langle \hat{\mathbf{u}}_h\cdot\hat\nu, \hat\mu\rangle_{\hat\Gamma^N} = \langle J_{\hat\nu}\hat g^N, \hat\mu\rangle_{\hat\Gamma^N}, \qquad \hat\mu \in \hat\Lambda_h^N, \tag{2.24}$$

where

$$J_{\hat\nu}(\hat{\mathbf{x}}) = J(\hat{\mathbf{x}})|(DF^{-1})^T\hat\nu|.$$

REMARK 2.1. We note that the geometry transformation always leads to a full computational tensor $JDF^{-1}K(DF^{-1})^T$, except in trivial cases, even if K is diagonal.

To obtain cell-centered finite differences on logically rectangular grids, we consider the lowest order Raviart-Thomas spaces [44] and take $\tilde{\mathbf{V}}_h = \mathbf{V}_h$. We employ quadrature rules to approximate the vector integrals in (2.21), (2.22). The two equations are replaced by

$$(\hat{\mathbf{u}}_h, \hat{\tilde{\mathbf{v}}})_{\hat\Omega,T} = \left(JDF^{-1}K(DF^{-1})^T\hat{\tilde{\mathbf{u}}}_h, \hat{\tilde{\mathbf{v}}}\right)_{\hat\Omega,T}, \qquad \hat{\tilde{\mathbf{v}}} \in \hat{\tilde{\mathbf{V}}}_h, \tag{2.25}$$

$$\begin{aligned}(\hat{\tilde{\mathbf{u}}}_h, \hat{\mathbf{v}})_{\hat\Omega,T} - (\hat p_h, \hat\nabla\cdot\hat{\mathbf{v}})_{\hat\Omega} & \qquad\qquad (2.26)\\ = -\langle \hat g^D, \hat{\mathbf{v}}\cdot\hat\nu\rangle_{\hat\Gamma^D} - \langle\hat\lambda_h, \hat{\mathbf{v}}\cdot\hat\nu\rangle_{\hat\Gamma^N}, &\qquad \hat{\mathbf{v}} \in \hat{\mathbf{V}}_h,\end{aligned}$$

where $(\,\cdot\,,\,\cdot\,)_{S,T}$ denote an application of the trapezoidal rule to the $L^2(S)$ inner product with respect to $\hat{\mathcal{T}}_h$.

This choice of quadrature rules gives diagonal coefficient matrices for $\hat{\mathbf{u}}_h$ in (2.25) and for $\hat{\tilde{\mathbf{u}}}_h$ in (2.26). Therefore the vector unknowns can be eliminated, leading to cell-centered finite differences for the pressure with 9 point stencil in two dimensions and 19 point stencil in three dimensions.

The following convergence result can be found in [1, 4].

THEOREM 2.2. *Let Ω^* be a fixed domain compactly contained in Ω. For the cell-centered finite difference method* (2.25), (2.26), (2.23), (2.24) *on logically rectangular grids, if $p \in C^{3,1}(\bar\Omega)$, $\mathbf{u} \in \left(C^1(\bar\Omega)\bigcap W^{2,\infty}(\Omega)\right)^d$, and $K \in \left(C^1(\bar\Omega_i)\bigcap W^{2,\infty}(\Omega_i)\right)^{d\times d}$, then there exists a constant C, independent of h but dependent on the solution and K as indicated , and on $\|F\|_{3,\infty,\Omega}$, and $\|F^{-1}\|_{3,\infty,\Omega}$, such that*

$$\|\mathbf{u}-\mathbf{u}_h\|_M + \|\tilde{\mathbf{u}}-\tilde{\mathbf{u}}_h\|_M \le Ch^{3/2}, \tag{2.27}$$

$$\|\mathbf{u}-\mathbf{u}_h\|_{M,\Omega^*} + \|\tilde{\mathbf{u}}-\tilde{\mathbf{u}}_h\|_{M,\Omega^*} \le Ch^2, \tag{2.28}$$

$$\|\nabla\cdot(\mathbf{u}-\mathbf{u}_h)\|_M \le Ch^2, \tag{2.29}$$

$$\|p-p_h\|_M \le Ch^2. \tag{2.30}$$

Here $(\cdot,\cdot)_M$ is an application of the midpoint rule and $\|\cdot\|_M = (\cdot,\cdot)_M^{1/2}$.

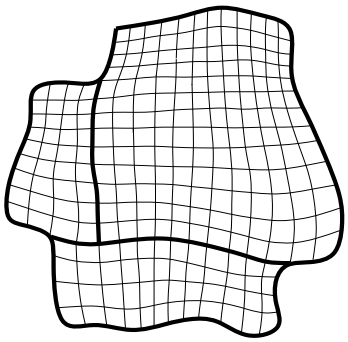

FIG. 1. *Multiblock domain*

REMARK 2.2. Theorem 2.2 implies superconvergence in L^2 for the computed pressure, velocity and its divergence at the midpoints of the elements. The velocity exhibits full $O(h^2)$ superconvergence away from the boundary. The loss of half a power of h for the velocity in (2.27) is due to the $O(h)$ approximation on $\partial\Omega$.

Computational results confirm the theoretical results of Theorem 2.2. The method has been implemented in a single phase flow 3-D simulator ParFlow1 developed by the Subsurface Modeling Group at Rice University [22]. The code runs on massively parallel distributed memory computers. A substructuring domain decomposition algorithm by Glowinski and Wheeler [36, 24] is used in the solver. Balancing preconditioner developed by Cowsar, Mandel, and Wheeler allows for ill-conditioned problems with several orders of magnitude variation in the permeability to be handled very efficiently.

A cell-centered finite difference scheme on triangular meshes based on the expanded mixed formulation have also been developed and analyzed in [1]. It has been implemented in the Rice Unstructured Flow code [37], which can handle coupled unstructured and logically rectangular grids.

A locally mass conservative characteristics-mixed method has been developed by Arbogast and Wheeler [3] for solving advection-dominated transport problems. The expanded mixed method combined with the characteristics-mixed method has been used for accurate and efficient approximation of transport problems on general geometry domains [5].

2.3. The expanded mixed method for problems with discontinuous coefficients on multiblock domains. The results of the previous section require the permeability K and the mapping F to be smooth functions. In many applications this is not the case. The permeability of heterogeneous media can be discontinuous. On the other hand, very irregular domains are difficult to map to a regular shape domain via smooth mappings. In those cases, multiblock structure has to be used, with different mappings for the different blocks. Therefore the global map is piecewise smooth and could be non-differentiable across the interfaces (see Figure 1).

Computational results in [2, 1] indicate loss of convergence along interfaces of map or coefficient discontinuities. Note that the transformed computational tensor is

$$\mathcal{K} = JDF^{-1}K(DF^{-1})^T,$$

so a nonsmooth mapping leads to a discontinuous coefficient on the reference domain. This implies discontinuous pressure gradient. In the above finite difference scheme

however, $\hat{\tilde{\mathbf{u}}}_h = \hat{\nabla}\hat{p}_h$ is continuous in the normal direction. This inconsistency causes the loss of convergence along the discontinuities.

To correct for the above problem, we need to relax the continuity constraints for $\tilde{\mathbf{V}}_h$ across the interfaces. Pressure Lagrange multipliers are introduced there, leading to a partially hybridized mixed formulation. Assume that Ω can be decomposed into a set of non-intersecting subdomains $\Omega_i, 1 \le i \le n$, and the restrictions of K and F to any subdomain are smooth functions. The following weak form can be obtained by integrating over each Ω_i and summing.

$$(M\mathbf{u}, \tilde{\mathbf{v}}) = (MKM\tilde{\mathbf{u}}, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in (L^2(\Omega))^d, \tag{2.31}$$

$$(M\tilde{\mathbf{u}}, \mathbf{v}) = \sum_{i=1}^{n} \left\{ (p, \nabla\cdot\mathbf{v})_{\Omega_i} - \langle \lambda, \mathbf{v}\cdot\nu\rangle_{\partial\Omega_i\setminus\Gamma^D} \right\} \tag{2.32}$$

$$- \langle g^D, \mathbf{v}\cdot\nu\rangle_{\Gamma^D}, \qquad \mathbf{v} \in \bigcup_{i=1}^{n} H(\mathrm{div};\Omega_i),$$

$$\sum_{i=1}^{n} (\nabla\cdot\mathbf{u}, w)_{\Omega_i} = (f, w), \qquad w \in L^2(\Omega), \tag{2.33}$$

$$\sum_{i=1}^{n} \langle \mathbf{u}\cdot\nu, \mu\rangle_{\partial\Omega_i\setminus\Gamma^D} = \langle g^N, \mu\rangle_{\Gamma^N}, \qquad \mu \in H^{1/2}(\Gamma\setminus\Gamma^D), \tag{2.34}$$

where $\Gamma = \bigcup_{i=1}^{n} \partial\Omega_i$.

Let $\mathcal{T}_h^i$ be a partition of Ω_i, $1 \le i \le n$, and let this partitions match on the interfaces of the subdomains. Let $\mathbf{V}_h^i \times W_h^i \subset H(\mathrm{div};\Omega_i) \times L^2(\Omega_i)$ be any mixed spaces on Ω_i. Let $\mathbf{V}_h^* = \bigcup_{i=1}^{n} \mathbf{V}_h^i$, $\tilde{\mathbf{V}}_h^* = \bigcup_{i=1}^{n} \tilde{\mathbf{V}}_h^i$, $W_h^* = \bigcup_{i=1}^{n} W_h^i$, and Λ_h^* denote the Lagrange multiplier space on $\Gamma\setminus\Gamma^D$ associated with $\mathbf{V}_h^* \times W_h^*$. We then solve for $\mathbf{u}_h \in \mathbf{V}_h^*$, $\tilde{\mathbf{u}}_h \in \tilde{\mathbf{V}}_h^*$, $p_h \in W_h^*$, and $\lambda_h \in \Lambda_h^*$ satisfying

$$(M\mathbf{u}_h, \tilde{\mathbf{v}}) = (MKM\tilde{\mathbf{u}}_h, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_h^*, \tag{2.35}$$

$$(M\tilde{\mathbf{u}}_h, \mathbf{v}) = \sum_{i=1}^{n} \left\{ (p_h, \nabla\cdot\mathbf{v})_{\Omega_i} - \langle \lambda_h, \mathbf{v}\cdot\nu\rangle_{\partial\Omega_i\setminus\Gamma^D} \right\} \tag{2.36}$$

$$- \langle g^D, \mathbf{v}\cdot\nu\rangle_{\Gamma^D}, \qquad \mathbf{v} \in \mathbf{V}_h^*,$$

$$\sum_{i=1}^{n} (\nabla\cdot\mathbf{u}_h, w)_{\Omega_i} = (f, w), \qquad w \in W_h^*, \tag{2.37}$$

$$\sum_{i=1}^{n} \langle \mathbf{u}_h\cdot\nu, \mu\rangle_{\partial\Omega_i\setminus\Gamma^D} = \langle g^N, \mu\rangle_{\Gamma^N}, \qquad \mu \in \Lambda_h^*. \tag{2.38}$$

Following [1] we refer to (2.35)–(2.38) as the enhanced method. Note that the flux-matching condition (2.38) guarantees that $\mathbf{u}_h \in H(\mathrm{div};\Omega)$, while $\tilde{\mathbf{u}}_h$ is discontinuous across the subdomain interfaces. Let $\mathbf{V}_h^i \times W_h^i$ be the RT_0 spaces on Ω_i. Use of quadrature rules as in Section 2.2 leads to a sparse symmetric positive definite system for p_h and λ_h. The stencil is slightly modified only near the interfaces where Lagrange multipliers are added. Therefore the computational cost for the enhanced method is compatible with the one for the expanded method. Moreover, the Glowinski-Wheeler domain decomposition algorithm [36, 24] can be used to solve the linear system. There,

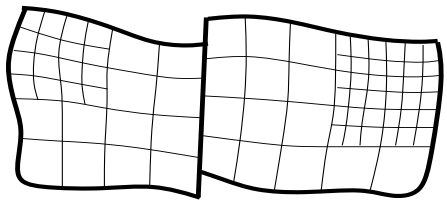

FIG. 2. *Grid around a fault and locally refined grid*

Lagrange multipliers are introduced on subdomain interfaces for a purpose of parallelism, so the solution to the enhanced method comes at no extra cost.

Computational results in [2, 1] show that convergence along the discontinuities is regained for the enhanced method. Using techniques similar to those used in [4, 1] we can show the following result.

THEOREM 2.3. *For the cell-centered finite difference approximation of the enhanced mixed method* (2.35)–(2.38) *on a logically rectangular grid, if* $p \in C^{3,1}(\bar{\Omega}_i) \bigcap C^0(\bar{\Omega})$, $\mathbf{u} \in \left(C^1(\bar{\Omega}_i) \bigcap W^{2,\infty}(\Omega_i)\right)^d \bigcap H(\mathrm{div};\Omega)$, *and* $K \in \left(C^1(\bar{\Omega}_i) \bigcap W^{2,\infty}(\Omega_i)\right)^{d\times d}$, *then there exists a constant* C, *independent of* h *but dependent on the solution and* K *as indicated , and on* $\|F\|_{3,\infty,\Omega_i}$, $\|F^{-1}\|_{3,\infty,\Omega_i}$, $\|DF\|_{0,\infty}$, *and* $\|DF^{-1}\|_{0,\infty}$, *such that*

$$\|\mathbf{u} - \mathbf{u}_h\|_M + \|\tilde{\mathbf{u}} - \tilde{\mathbf{u}}_h\|_M \le Ch^{3/2}, \tag{2.39}$$

$$\|\nabla \cdot (\mathbf{u} - \mathbf{u}_h)\|_M \le Ch^2, \tag{2.40}$$

$$\|p - p_h\|_M \le Ch^2. \tag{2.41}$$

In many applications the geometry of the domain or the behavior of the solution may require using different grids in different parts of the domain. This is the case with porous media problems in a presence of faults. Local refinement techniques are also widely used for accurate and computationally efficient approximation of local phenomena (e.g. high gradients around the wells). The type of grid used in such cases is shown on Figure 2.

The partially hybridized form of the mixed method is also needed for solving problems on non-matching or locally refined grids.

Let us assume that Ω can be decomposed into subdomains $\{\Omega_i\}_{i=1}^n$ such that all faults lie along the interfaces. Thus the grids are smooth within each subdomain and possibly non-matching on the subdomain boundaries.

In this setting we again have the expanded variational form (2.31)–(2.34) and its hybrid-mixed finite element approximation (2.35)–(2.38) with the only difference in the definition of Λ_h^*. To define it we use the idea of mortar boundary elements. This method has been analyzed in [10] for coupling of Galerkin finite elements and spectral discretizations. For any edge $\gamma_{ij} = \partial\Omega_i \bigcap \partial\Omega_j$ we define $\Lambda_h^*(\gamma_{ij})$ to be the normal trace of either $\mathbf{V}_h^i$ or $\mathbf{V}_h^j$. In other words, $\Lambda_h^*(\gamma_{ij})$ is the space of pressure Lagrange multipliers associated with one of these velocity spaces (see Figure 3 for RT_0 case). Note that, because of the non-conformity of the grids, the continuity condition (2.38) only implies that the fluxes match in an average sense on any element of the boundary grid. We observe that the mixed mortar finite element method is nothing else but the hybrid mixed method on non-matching grids.

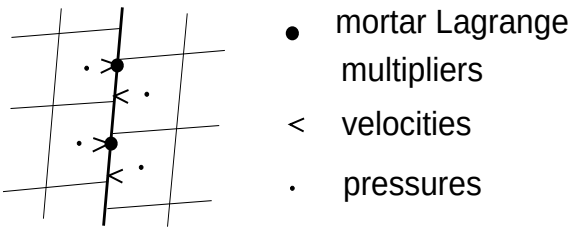

FIG. 3. *Non-matching grids along a segment of a fault, mortar Lagrange multipliers*

Locally refined grids can be viewed as a special case of non-matching grids, thus the technique discussed above is also applicable in this case. Computational experiments by Cowsar [22, 19] indicate that the mortar approach on locally refined grids possesses good approximation properties. Note that our approach differs from the previous works on mixed methods with local refinement [31, 40, 35], where the notion of "slave" velocities is used.

We close the section with a remark that all of the above schemes can be implemented very efficiently, using the domain decomposition techniques proposed by Glowinski and Wheeler [36, 24] with balancing preconditioning [21], or the parallel multigrid algorithm developed by Cowsar, Weiser, and Wheeler [23]. These methods require only subdomain linear solves, where the grids are regular and structured, with possible slight modification of the computational stencil near the interfaces. Recently Kuznetsov and Wheeler [39] used the Lagrange multiplier formulation to construct optimal substructuring preconditioners for mixed methods on non-matching grids.

3. Mixed finite element methods for multiphase flow. In this section we consider mixed finite element discretizations for the coupled nonlinear system of multiphase flow equations. We consider an immiscible two-phase flow model. Extensions to three or more phases are straightforward. The governing equations for fluid motion through porous medium are mass conservation of phases [8, 15]

$$\frac{\partial(\phi s_i \rho_i)}{\partial t} + \nabla \cdot (\rho_i \mathbf{u}_i) = q_i, \quad (\mathbf{x}, t) \in \Omega \times (0, T), \tag{3.1}$$

where $i = w$ (wetting), n (non-wetting) denotes the phase, s_i is the phase saturation, ρ_i is the phase density, ϕ is the porosity, q_i is the source term, and

$$\mathbf{u}_i = -\frac{k_i(s_i)K}{\mu_i}(\nabla p_i - \rho_i g \nabla D), \quad (\mathbf{x}, t) \in \Omega \times (0, T), \tag{3.2}$$

is the Darcy velocity. Here p_i is the phase pressure, K is the absolute permeability tensor, $k_i(s_i)$ is the phase relative permeability, μ_i is the phase viscosity, g is the gravitational constant, and D is the depth. The two equations are coupled with the volume balance equation

$$s_w + s_n = 1$$

and the capillary pressure relation

$$p_c(s_w) = p_n - p_w.$$

No flow boundary conditions

$$\mathbf{u}_i \cdot \nu = 0, \quad (\mathbf{x}, t) \in \partial\Omega \times (0, T)$$

are considered only for simplicity. Initial condition

$$s_w(\mathbf{x}, 0) = s_0(\mathbf{x}), \quad \mathbf{x} \in \Omega,$$

completes the model.

For simplicity of the presentation we restrict our discussion to incompressible fluids and media, i.e. constant densities and porosity, and neglect gravity effects.

REMARK 3.1. The relative permeabilities $k_i(s_i)$ vanish at $s_i = 0$, $i = w, n$ (see [9]), making the equations (3.1) degenerate . This causes difficulties in the analysis of the numerical method.

3.1. The expanded mixed method for multiphase flow. As in Section 2, we introduce the pressure gradients

$$\tilde{\mathbf{u}}_i = -\nabla p_i, \quad i = w, n.$$

Then

$$\mathbf{u}_i = \lambda_i(s) K \tilde{\mathbf{u}}_i,$$

where $\lambda_i = k_i/\mu_i$ is the phase mobility and $s = s_w$. We omit the geometry factor M for simplicity. General geometry domains are handled in the same way as in the single flow case.

Define

$$\mathbf{V} = \{\mathbf{v} \in H(\mathrm{div}; \Omega) : \mathbf{v} \cdot \nu = 0 \text{ on } \partial\Omega\}.$$

In the expanded mixed variational form we seek, for every time $t \in [0, T]$, $\mathbf{u}_i(\cdot, t) \in \mathbf{V}$, $\tilde{\mathbf{u}}_i(\cdot, t) \in (L^2(\Omega))^d$, $p_i(\cdot, t) \in L^2(\Omega)$, $i = w, n$, and $s(\cdot, t) \in L^2(\Omega)$ such that

$$(\mathbf{u}_i, \tilde{\mathbf{v}}) = (\lambda(s) K \tilde{\mathbf{u}}_i, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in (L^2(\Omega))^d, \tag{3.3}$$

$$(\tilde{\mathbf{u}}_i, \mathbf{v}) - (p_i, \nabla \cdot \mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}, \tag{3.4}$$

$$\phi(\frac{\partial s}{\partial t}, w) + (\nabla \cdot \mathbf{u}_w, w) = (\tilde{q}_w(s), w), \qquad w \in L^2(\Omega), \tag{3.5}$$

$$-\phi(\frac{\partial s}{\partial t}, w) + (\nabla \cdot \mathbf{u}_n, w) = (\tilde{q}_n(s), w), \qquad w \in L^2(\Omega), \tag{3.6}$$

$$(p_n - p_w, w) = (p_c(s), w), \qquad w \in L^2(\Omega), \tag{3.7}$$

$$(s(\cdot, 0), w) = (s_0, w), \qquad w \in L^2(\Omega), \tag{3.8}$$

where $\tilde{q}_i = q_i/\rho_i$.

REMARK 3.2. As in the single flow case, the expanded mixed formulation allows us to handle efficiently full permeability tensor. There is one more reason the expanded form is used here. The phase mobility $\lambda_i(s_i)$ vanishes at $s_i = 0$. The standard mixed method requires inverting the coefficient $\lambda_i(s)K$, which is impossible when $\lambda_i(s) = 0$.

Let $\mathcal{T}_h$ be a finite element partition of Ω, where h is associated with the size of the elements. Let $\mathbf{V}_h \times W_h \subset \mathbf{V} \times L^2(\Omega)$ be any of the known mixed finite element spaces on $\mathcal{T}_h$.

Let $\tilde{\mathbf{V}}_h$ be a finite element subspace of $(L^2(\Omega))^d$ such that $\mathbf{V}_h \subseteq \tilde{\mathbf{V}}_h$.

Let $\{t_n\}_{n=0}^N$ be a partition of $[0,T]$ with $t_0 = 0$ and $t_N = T$, let $\Delta t^n = t_n - t_{n-1}$, and let $f^n = f(t_n)$.

We have the following backward Euler expanded mixed finite element method for the multiphase flow system. Find, for any $0 \le n \le N$, $(\mathbf{u}_{i,h}^n, \tilde{\mathbf{u}}_{i,h}^n, p_{i,h}^n) \in \mathbf{V}_h \times \tilde{\mathbf{V}}_h \times W_h$, $i = w, n$, and $s_h^n \in W_h$ such that

$$(\mathbf{u}_{i,h}^n, \tilde{\mathbf{v}}) = (\lambda(s_h^n) K \tilde{\mathbf{u}}_{i,h}^n, \tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_h, \tag{3.9}$$

$$(\tilde{\mathbf{u}}_{i,h}^n, \mathbf{v}) - (p_{i,h}^n, \nabla \cdot \mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}_h, \tag{3.10}$$

$$\phi(\frac{s_h^n - s_h^{n-1}}{\Delta t^n}, w) + (\nabla \cdot \mathbf{u}_{w,h}^n, w) = (\tilde{q}_w(s_h^n), w), \qquad w \in W_h, \tag{3.11}$$

$$-\phi(\frac{s_h^n - s_h^{n-1}}{\Delta t^n}, w) + (\nabla \cdot \mathbf{u}_{n,h}^n, w) = (\tilde{q}_n(s_h^n), w), \qquad w \in W_h, \tag{3.12}$$

$$(p_{n,h}^n - p_{w,h}^n, w) = (p_c(s_h^n), w), \qquad w \in W_h, \tag{3.13}$$

$$(s_h^0, w) = (s_0, w), \qquad w \in W_h. \tag{3.14}$$

REMARK 3.3. The choice of fully implicit time discretization is motivated by the fact that all known explicit or partially implicit schemes suffer from severe time step stability limitations when advection processes are dominating.

Use of trapezoidal quadrature rule for approximating the vector inner products in (3.9), (3.10) allows the vector unknowns to be eliminated. One of the phase pressures can be further eliminated using the capillary pressure equation (3.13). Thus a coupled cell-centered finite difference system for one pressure and one saturation is obtained. The stencil for the pressures or the saturations is 5 points for $d = 2$ and 7 points for $d = 3$ if K is diagonal, and 9 points for $d = 2$ and 19 points for $d = 3$ if K is a full tensor.

REMARK 3.4. The cell-centered finite difference scheme described above has been commonly used by the environmental and petroleum engineers [43, 8]. It conserves the mass of all phases locally. The mixed finite element formulation provides more robustness for handling irregular geometries and general boundary conditions, and is useful in the convergence analysis.

REMARK 3.5. The use of quadrature rule requires evaluation of $\lambda_i(s_h)$ on the edges. Since s_h is constant on any element, $\lambda_i(s_h)$ along the edges cannot be directly computed. One-point upstream weighting is used to determine these values. This choice further stabilize the method.

The above finite difference scheme has been originally implemented in a two-phase flow three dimensional simulator ParFlow2 developed by John A. Wheeler of Exxon Production Research Company and modified by the Subsurface Modeling Group at Rice University. The code runs on distributed memory parallel machines. It handles slightly compressible flow and has been successfully used in black oil and ground water applications.

Recently a new optimization approach for solving the finite difference equations has been introduced [20]. The algorithm requires only symmetric positive definite linear solves, thus taking advantage of the wide variety of efficient and robust solvers available.

3.2. Mixed methods based on the fractional flow formulation. It has been a common approach to reformulate the two-phase flow system as a pressure equation of elliptic or parabolic type and a saturation equation of advection-diffusion type. This formulation has certain advantages in the analysis of the numerical methods. In this section we present the expanded mixed finite element method for the fractional flow formulation and show that it preserves the local mass conservation properties of the scheme from the previous section.

Let

$$\lambda = \lambda_w + \lambda_n$$

be the total mobility and let

$$\mathbf{u} = \mathbf{u}_w + \mathbf{u}_n$$

be the total velocity. Multiplying (3.1) by $1/\rho_i$ and adding them together, we get

$$\nabla \cdot \mathbf{u} = q, \tag{3.15}$$

where $q = q_w/\rho_w + q_n/\rho_n$. Let us define the global pressure to be

$$p = p_w + \int_0^{p_c(s)} \left(\frac{\lambda_n}{\lambda}\right)\left(p_c^{-1}(\zeta)\right) d\zeta.$$

Thus

$$\mathbf{u} = -\lambda K \nabla p. \tag{3.16}$$

Equation (3.15) is referred to as the pressure equation. Since $\lambda > 0$ and K is a symmetric positive definite tensor, this is an elliptic equation. For compressible flow the pressure equation is parabolic.

To derive the saturation equation, we first observe that

$$\frac{\lambda_w}{\lambda}\mathbf{u} = \mathbf{u}_w - \frac{\lambda_w \lambda_n}{\lambda} K \nabla p_c(s).$$

Substituting this expression into the water conservation equation (3.1), we get the saturation equation

$$\phi \frac{\partial s}{\partial t} + \nabla \cdot \Big(\beta(s)\mathbf{u} + \alpha(s) K \nabla p_c(s)\Big) = \tilde{q}_w, \tag{3.17}$$

where $\beta(s) = \lambda_w/\lambda$, $\alpha(s) = \lambda_w \lambda_n/\lambda$, and $\tilde{q}_w = q_w/\rho_w$. Note that $p_c(s)$ is a strictly monotone decreasing function. We can write the last term on the left in (3.17) as

$$\alpha(s) K \frac{\partial p_c}{\partial s} \nabla s \equiv -\sigma(s) K \nabla s.$$

Therefore (3.17) is an advection-diffusion equation. The diffusion term vanishes at $s = 0, 1$ - the minimum and maximum values of the saturation. This is due to the behavior of the relative permeability and the capillary pressure functions (see [9]).

One possible technique to handle the degenerate diffusion term is to use the Kirchoff transformation. Let

$$D(s) = \int_0^s \sigma(\zeta)\, d\zeta.$$

Then

$$\nabla D(s) = \sigma(s)\nabla s,$$

and the saturation equation becomes

$$\phi\frac{\partial s}{\partial t} + \nabla\cdot\Big(\beta(s)\mathbf{u} - K\nabla D(s)) = \tilde{q}_w. \tag{3.18}$$

In [6] Arbogast, Wheeler and Zhang analyze a mixed finite element method for equation (3.18). They assume that the total velocity $\mathbf{u}$ is given and obtain optimal error bounds.

To obtain the expanded mixed variational formulation of (3.15), (3.18) we introduce the variables

$$\tilde{\mathbf{u}} = -\nabla p, \tag{3.19}$$
$$\tilde{\psi} = -\nabla D(s), \tag{3.20}$$
$$\psi = \beta(s)\mathbf{u} + K\tilde{\psi} \equiv \mathbf{u}_w. \tag{3.21}$$

We now have, for every time $t \in [0,T]$, the variational form for $\mathbf{u}(\cdot,t) \in \mathbf{V}$, $\tilde{\mathbf{u}}(\cdot,t) \in (L^2(\Omega))^d$, and $p(\cdot,t) \in L^2(\Omega)$ as

$$(\mathbf{u},\tilde{\mathbf{v}}) = (\lambda(s)K\tilde{\mathbf{u}},\tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in (L^2(\Omega))^d, \tag{3.22}$$
$$(\tilde{\mathbf{u}},\mathbf{v}) - (p,\nabla\cdot\mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}, \tag{3.23}$$
$$(\nabla\cdot\mathbf{u},w) = (q(s),w), \qquad w \in L^2(\Omega), \tag{3.24}$$

and the variational form for $\psi(\cdot,t) \in \mathbf{V}$, $\tilde{\psi}(\cdot,t) \in (L^2(\Omega))^d$, and $s(\cdot,t) \in L^2(\Omega)$ as

$$(\psi,\tilde{\mathbf{v}}) = (\beta(s)\mathbf{u},\tilde{\mathbf{v}}) + (K\tilde{\psi},\tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in (L^2(\Omega))^d, \tag{3.25}$$
$$(\tilde{\psi},\mathbf{v}) - (D(s),\nabla\cdot\mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}, \tag{3.26}$$
$$(\frac{\partial s}{\partial t},w) + (\nabla\cdot\psi,w) = (\tilde{q}_w(s),w), \qquad w \in L^2(\Omega), \tag{3.27}$$
$$(s(\cdot,0),w) = (s_0,w), \qquad w \in L^2(\Omega). \tag{3.28}$$

With the finite element and time discretization notation from Section 3.1, we have the following backward Euler mixed finite element approximation to (3.22)–(3.28). For any $0 \le n \le N$, find $(\mathbf{u}_h^n, \tilde{\mathbf{u}}_h^n, p_h^n) \in \mathbf{V}_h \times \tilde{\mathbf{V}}_h \times W_h$ such that

$$(\mathbf{u}_h^n,\tilde{\mathbf{v}}) = (\lambda(s_h^n)K\tilde{\mathbf{u}}_h^n,\tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_h, \tag{3.29}$$
$$(\tilde{\mathbf{u}}_h^n,\mathbf{v}) - (p_h^n,\nabla\cdot\mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}_h, \tag{3.30}$$
$$(\nabla\cdot\mathbf{u}_h^n,w) = (q(s_h^n),w), \qquad w \in W_h, \tag{3.31}$$

and $(\psi_h^n, \tilde{\psi}_h^n, s_h^n) \in \mathbf{V}_h \times \tilde{\mathbf{V}}_h \times W_h$ such that

$$(\psi_h^n,\tilde{\mathbf{v}}) = (\beta(s_h^n)\mathbf{u}_h^n,\tilde{\mathbf{v}}) + (K\tilde{\psi}_h^n,\tilde{\mathbf{v}}), \qquad \tilde{\mathbf{v}} \in \tilde{\mathbf{V}}_h, \tag{3.32}$$
$$(\tilde{\psi}_h^n,\mathbf{v}) - (D(s_h^n),\nabla\cdot\mathbf{v}) = 0, \qquad \mathbf{v} \in \mathbf{V}_h, \tag{3.33}$$
$$\left(\frac{s_h^n - s_h^{n-1}}{\Delta t^n},w\right) + (\nabla\cdot\psi_h^n,w) = (\tilde{q}_w(s_h^n),w), \qquad w \in W_h, \tag{3.34}$$
$$(s_h^0,w) = (s_0,w), \qquad w \in W_h. \tag{3.35}$$

REMARK 3.6. Equation (3.34) is a locally mass conservative approximation of the water conservation equation (note that by construction $\psi = \mathbf{u}_w$). Subtracting (3.34) from (3.31) we get

$$-\left(\frac{s_h^n - s_h^{n-1}}{\Delta t^n}, w\right) + (\nabla \cdot (\mathbf{u}_h^n - \psi_h^n), w) = (\tilde{q}_n(s_h^n), w), \quad w \in W_h, \tag{3.36}$$

which is an element by element approximation to the oil conservation equation, so the scheme conserves the mass of both phases locally. Therefore the mixed method for the pressure-saturation formulation preserves the conservation properties of the cell-centered finite difference scheme applied directly to the phase conservation equations and described in the previous section.

REMARK 3.7. If the permeability tensor is discontinuous, or the domain has multiblock structure with non-smooth grids across the interfaces, the hybrid form of the expanded mixed method has to be used. Following Section 2.3, we can introduce Lagrange multipliers for p and s along the discontinuities. Note that this also allows us to handle p_c varying discontinuously in space. The techniques discussed in Section 2.3 for approximations on non-matching and locally refined grids can also be extended to the multiphase flow system.

4. Some conclusions and current research. We have discussed mixed finite element methods for modeling flow and transport in porous media. The theoretical and computational results indicate that the mixed methods are accurate, robust, and efficient numerical tool for porous media applications. Their main advantage is local mass conservation, continuity of fluxes, and good approximation of both pressure and velocity. The methods discussed in the paper can handle full tensor permeabilities, domains with irregular geometries, including multiblock domains, discontinuous coefficients, and non-matching grids. They can be implemented as cell-centered finite differences and require regular data structure (logically rectangular grids); therefore they can be easily incorporated into existing simulators.

The current research includes analysis of the presented numerical schemes for the multiphase flow system and development of new solvers and preconditioners for non-symmetric and indefinite linear systems arising in the discretizations of the nonlinear partial differential equations.

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