THE APPLICATION OF MIXED METHODS TO SUBSURFACE SIMULATION

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SUMMARY

We consider the application of mixed finite element and finite difference methods to groundwater flow and transport problems. We are concerned with accurate approximation and efficient implementation, especially when the porous medium may have geometric irregularities, heterogeneities, and either a tensor hydraulic conductivity or a tensor dispersion. For single-phase flow, we develop an expanded mixed finite element method defined on a logically rectangular, curvilinear grid. Special quadrature rules are introduced to transform the method into a simple cell-centered finite difference method. The approximation is locally conservative and highly accurate. We also show that the highly nonlinear two-phase flow problem is well approximated by mixed methods. The main difficulty is that the true solution is typically lacking in regularity.

INTRODUCTION

Our primary goal is to develop discretization methods that accurately and efficiently approximate the equations governing subsurface multi-phase flow and transport. We can judge the accuracy of an approximation by many criteria. Asymptotic convergence results tell us that we have an accurate solution when the mesh spacing h is *small enough*. Often, we cannot use as fine a mesh resolution as we would like, because of the computational effort needed to solve the equations. An equally important criterion to consider is the ability of the numerical scheme to preserve important qualitative properties of the governing equations so that physically meaningful results are obtained on a relatively coarse discretization scale. The most important qualitative property in subsurface simulation is conservation of mass. Mass should be conserved locally, that is, element-by-element.

Several additional physical phenomena need to be addressed by our numerical schemes. They should handle tensor permeabilities and dispersivities. Dispersivities are naturally tensors, and tensor permeabilities can arise from the use of homogenization or scale-up techniques. Subsurface aquifers are irregularly shaped and contain layers with differing material properties. Nonlinear effects are also prevalent especially in multi-phase flow.

We present here some of our work on mixed finite element and finite difference methods [9, 6, 10, 5, 8, 4, 7]. These methods are "mixed" in that they approximate directly *both* pressure and velocity (in the flow problem), and they are asymptotically accurate and conserve mass locally. The standard mixed finite element method was developed by Raviart and Thomas [19, 21, 12], and we restrict our attention to their lowest-order method. It was

first used to solve subsurface problems by Douglas, Ewing, and Wheeler [14], although Russell and Wheeler [20] pointed out that the often used cell-centered finite difference method on rectangular grids [18] for problems with diagonal permeabilities is the lowest order Raviart-Thomas mixed finite element method approximated by applying appropriate quadrature rules to some of the integrals.

A problem with mixed methods that we address is that they can be difficult to implement directly, especially if the aquifer domain is not rectangular or the permeability is a tensor. There has also been very little theoretical basis for concluding that the approximation of highly nonlinear multi-phase problems is accurate.

Our discretization schemes are based on an expanded mixed finite element method that we define below. An approximation to this expanded mixed method reduces it to cell-centered finite differences; thus, it is easy to implement and has only one unknown per element. The elements can be deformed rectangles or bricks, although many of our results extend to triangles and tetrahedra [6].

FINITE ELEMENT APPROXIMATION OF SINGLE-PHASE FLOW

To illustrate the numerical schemes, we begin by considering incompressible, single phase subsurface flow on the aquifer domain $\Omega \subset \mathbf{R}^d$, $d = 2$ or 3. We solve for the pressure p and the velocity $\mathbf{u}$ satisfying

$$\mathbf{u} = -\mathbf{K}\nabla p, \quad \mathbf{x} \in \Omega, \tag{1}$$

$$\nabla \cdot \mathbf{u} = q, \quad \mathbf{x} \in \Omega, \tag{2}$$

$$p = p_0, \quad \mathbf{x} \in \partial\Omega_D, \tag{3}$$

$$\mathbf{u} \cdot \nu = g, \quad \mathbf{x} \in \partial\Omega_N, \tag{4}$$

where $\mathbf{K}$ is the hydraulic conductivity tensor, q is a source term, ν is the outer unit normal vector to $\partial\Omega$, p_0 gives a Dirichlet boundary condition on $\partial\Omega_D$, and g gives a Neumann condition. This is a second order elliptic equation.

Lowest order Raviart-Thomas spaces.

Let $L^2(\Omega)$ denote the space of square integrable functions, and let $H(\Omega;\mathrm{div})$ denote the space of vector functions that have a divergence; that is,

$$L^2(\Omega) = \left\{ w(\mathbf{x}) : \int_\Omega |w|^2 \, dx < \infty \right\},$$
$$H(\Omega;\mathrm{div}) = \{\mathbf{v}(\mathbf{x}) : \mathbf{v} \in (L^2(\Omega))^d \text{ and } \nabla \cdot \mathbf{v} \in L^2(\Omega)\}.$$

We suppose that the domain Ω is partitioned into a finite number of non-overlapping elements or cells E of maximal diameter h. In the lowest order Raviart-Thomas mixed spaces [19, 16, 11], pressures can be approximated over elements or on element faces (or edges in 2-D). Element pressures are approximated in

$$W_h = \{w : w \text{ is constant on each element}\} \subset L^2(\Omega),$$

and, on the Neumann part of the exterior domain boundary, element face "Lagrange multiplier" pressures [11] are approximated in

$$\Lambda_h^N = \{\mu : \mu \text{ is constant on each element face of } \partial\Omega_N\} \subset L^2(\partial\Omega_N).$$

The nodal degrees of freedom can be considered as the function values at the centers of the elements or faces.

The velocity $\mathbf{u}$ is approximated in a space of vector valued functions $\mathbf{V}_h$ such that

$$\mathbf{V}_h \subset \{\mathbf{v} \in (L^2(\Omega))^d : \mathbf{v}\cdot\nu \text{ is constant on each element face and continuous across elements}\} \subset H(\Omega;\mathrm{div}).$$

On a 2-D (or 3-D) rectangle E, this space of functions is

$$\mathbf{V}_h|_E = \{\mathbf{v} : \mathbf{v}_i = a_i + b_i x_i \text{ for some constants } a_i \text{ and } b_i,\ i = 1, 2(, 3)\},$$

where we use the standard Cartesian decomposition of the vectors $\mathbf{x} = (x_1, x_2(, x_3))$ and $\mathbf{v} = (v_1, v_2(, v_3))$; that is, the ith component of $\mathbf{v}$ is linear in the ith coordinate direction and constant in the other direction(s). The important fact is that $\mathbf{v}\cdot\nu$ is a constant; therefore, the nodal degrees of freedom can be considered as the values of $\mathbf{v}\cdot\nu$ at the centers of the element faces.

For a relatively general shaped element E, assume that there is a map $F : \hat{E} \to E$ from a rectangle or brick $\hat{E}$ to E. Following Thomas [21], we use the Piola transform to define $\mathbf{V}_h|_E$ from $\hat{\mathbf{V}}_h|_{\hat{E}}$; this transform preserves normal fluxes in an average sense (i.e., it is locally mass conservative). Let the Jacobian matrix be $DF = (\partial F_i/\partial x_j)$. Then

$$\mathbf{v}(\mathbf{x}) = \frac{1}{J} DF\, \hat{\mathbf{v}}(\hat{\mathbf{x}}), \tag{5}$$

where $J = |\det(DF)|$.

The expanded mixed method.

Unlike the standard mixed method, we introduce a symmetric and positive definite tensor $\mathbf{G}$ and define the "adjusted" pressure gradient $\tilde{\mathbf{u}}$ by

$$\mathbf{G}\tilde{\mathbf{u}} = -\nabla p. \tag{6}$$

Then the system of equations is

$$\mathbf{K}\mathbf{G}\tilde{\mathbf{u}} - \mathbf{u} = 0, \tag{7}$$
$$\mathbf{G}\tilde{\mathbf{u}} + \nabla p = 0, \tag{8}$$
$$\nabla\cdot\mathbf{u} = q. \tag{9}$$

Denote inner-products over a set S by

$$(\varphi,\psi)_S = \int_S \varphi(\mathbf{x})\,\psi(\mathbf{x})\,d\mathbf{x} \quad \left(\text{or } \int_S \varphi(\mathbf{x})\cdot\psi(\mathbf{x})\,d\mathbf{x}\right),$$

and inner-products over a boundary set ∂S by

$$\langle\varphi,\psi\rangle_S = \int_{\partial S} \varphi(\mathbf{x})\,\psi(\mathbf{x})\,da(\mathbf{x}),$$

where S is omitted if $S = \Omega$. The expanded mixed finite element method is then: Find $\mathbf{u} \in \mathbf{V}_h$, $\tilde{\mathbf{u}} \in \mathbf{V}_h$, $p \in W_h$, and $\lambda \in \Lambda_h^N$ such that

$$(\mathbf{G}\mathbf{K}\mathbf{G}\tilde{\mathbf{u}}, \mathbf{v}) - (\mathbf{G}\mathbf{u}, \mathbf{v}) = 0 \quad \text{for all } \mathbf{v} \in \mathbf{V}_h, \tag{10}$$
$$(\mathbf{G}\tilde{\mathbf{u}}, \mathbf{v}) - (p, \nabla\cdot\mathbf{v}) = -\langle p_0, \mathbf{v}\cdot\nu\rangle_{\partial\Omega_D} - \langle\lambda, \mathbf{v}\cdot\nu\rangle_{\partial\Omega_N} \quad \text{for all } \mathbf{v} \in \mathbf{V}_h, \tag{11}$$
$$(\nabla\cdot\mathbf{u}, w) = (q, w) \quad \text{for all } w \in W_h, \tag{12}$$
$$\langle\mathbf{u}\cdot\nu, \mu\rangle_{\partial\Omega_N} = \langle g, \mu\rangle_{\partial\Omega_N} \quad \text{for all } \mu \in \Lambda_h. \tag{13}$$

We remark that if $\mathbf{G} = \mathbf{K}^{-1}$, then $\tilde{\mathbf{u}} = \mathbf{u}$ and we recover the standard mixed method [19, 21, 12]. If $\mathbf{G} = \mathbf{I}$, we recover the expanded mixed method considered in [24, 15, 13, 8, 9]. Later we will make a special choice of $\mathbf{G}$.

The algebraic system of equations that results is a symmetric saddle point linear system of the form

$$\begin{pmatrix} M & -A & 0 & 0 \\ -A^T & 0 & B & -L \\ 0 & B^T & 0 & 0 \\ 0 & -L^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \tilde{U} \\ U \\ P \\ \Lambda \end{pmatrix} = \begin{pmatrix} 0 \\ P_0 \\ Q \\ -G \end{pmatrix}, \tag{14}$$

where we represent $\mathbf{u}$ by U, $\tilde{\mathbf{u}}$ by $\tilde{U}$, p by P, and λ by Λ in the nodal bases $\{\mathbf{v}_i\}$ for $\mathbf{V}_h$, $\{w_i\}$ for W_h, and $\{\mu_i\}$ for Λ_h. In particular,

$$M_{ij} = (\mathbf{G}\mathbf{K}\mathbf{G}\mathbf{v}_i, \mathbf{v}_j) \quad \text{and} \quad A_{ij} = (\mathbf{G}\mathbf{v}_i, \mathbf{v}_j) \tag{15}$$

are symmetric and positive definite. To reduce the size of the linear system, we can solve for the Shur complement by eliminating

$$U = A^{-1}M\tilde{U} \quad \text{and} \quad \tilde{U} = A^{-1}(BP - L\Lambda - P_0) \tag{16}$$

to obtain

$$(\mathcal{B}A^{-1}MA^{-1}\mathcal{B}^T) \begin{pmatrix} P \\ \Lambda \end{pmatrix} = \begin{pmatrix} Q \\ -G \end{pmatrix} + (\mathcal{B}A^{-1}MA^{-1})P_0, \tag{17}$$

where $\mathcal{B} = \begin{pmatrix} B \\ L \end{pmatrix}$. This system is symmetric, positive definite, and relatively small (one unknown per element plus a few boundary nodes). Unfortunately, although A is sparse, A^{-1} is in general full. Iterative solution will require the following steps for the application of the matrix: a matrix vector multiply $x = \mathcal{B}^T \begin{pmatrix} P \\ \Lambda \end{pmatrix}$; the solution of the system $Ay = x$; and another matrix vector multiply $\mathcal{B}y$. Thus, we need inner iterations within our overall iterative solution, which can become somewhat expensive.

CELL-CENTERED FINITE DIFFERENCE APPROXIMATION

We now use approximate integration to reduce A in (17) to an easily inverted diagonal matrix.

The rectangular cell-centered finite difference approximation.

Assume in this subsection that the grid is rectangular. Take $\mathbf{G} = I$ and use the trapezoidal quadrature rule to approximate the first three integrals (i.e., those involving a vector-vector product) in (10)–(13). This diagonalizes the matrix A and the Shur complement system becomes sparse [20, 23], even when $\mathbf{K}$ is a tensor [8, 9].

It is easy to unravel the procedure in terms of the nodal degrees of freedom of $\mathbf{u}$, $\tilde{\mathbf{u}}$, p, and λ. Consider an element E (not adjacent to the outer boundary). Equation (12) requires that the divergence of $\mathbf{u}$ be set equal to the source term q. This involves differences of the normal velocities that live on the four edges or six faces of the element. Equation (10) relates the velocities to the gradients of pressure. The velocity $\mathbf{u}$ on a given

edge or face is related to the gradient $\tilde{\mathbf{u}}$ that lives on the given edge or face and to those that live on the adjacent but perpendicular four edges or eight faces (if $\mathbf{K}$ is not diagonal). Finally, (11) relates $\tilde{\mathbf{u}}$ living on an edge or face to the difference of the adjacent pressures. Combining this together, we get a 9 point stencil for the pressure on E if $d = 2$, and 19 points if $d = 3$. More details are given later and also in [9].

The Geometry Mapping.

To handle irregular geometry, we assume that there is a smooth mapping F of a rectangular, computational domain $\hat{\Omega}$ onto the domain Ω. Given a rectangular grid on $\hat{\Omega}$, F defines a smooth, logically rectangular, curvilinear grid on Ω. (In practice, there are grid generation codes available for creating F at the grid points. We use finite differences to approximate DF.)

The Transformed, Computational Problem.

In the expanded mixed method, take

$$\mathbf{G} = J(DF^{-1})^T DF^{-1}. \tag{18}$$

Transform (10)–(13) to the computational domain $\hat{\Omega}$. Vector and scalar basis functions transform by the Piola and natural transforms, respectively; that is,

$$\begin{aligned} \mathbf{v}(\mathbf{x}) &= \frac{1}{J(\hat{\mathbf{x}})} DF(\hat{\mathbf{x}})\hat{\mathbf{v}}(\hat{\mathbf{x}}) \qquad \text{(velocity)}, \\ w(\mathbf{x}) &= \hat{w}(\hat{\mathbf{x}}) \qquad\qquad\qquad\quad \text{(pressure)}. \end{aligned}$$

Thus we need to find $\hat{\mathbf{u}} \in \hat{\mathbf{V}}_h$, $\hat{\tilde{\mathbf{u}}} \in \hat{\mathbf{V}}_h$, $\hat{p} \in \hat{W}_h$, and $\hat{\lambda} \in \hat{\Lambda}_h$ such that

$$(\mathcal{K}\hat{\tilde{\mathbf{u}}}, \hat{\mathbf{v}}) = (\hat{\mathbf{u}}, \hat{\mathbf{v}}) \quad \text{for all } \hat{\mathbf{v}} \in \hat{\mathbf{V}}_h, \tag{19}$$

$$(\hat{\tilde{\mathbf{u}}}, \mathbf{v}) - (\hat{p}, \hat{\nabla} \cdot \hat{\mathbf{v}}) = -\langle \hat{p}_0, \hat{\mathbf{v}} \cdot \hat{\nu} \rangle_{\partial\hat{\Omega}_D} - \langle \hat{\lambda}, \hat{\mathbf{v}} \cdot \hat{\nu} \rangle_{\partial\hat{\Omega}_N} \quad \text{for all } \hat{\mathbf{v}} \in \hat{\mathbf{V}}_h, \tag{20}$$

$$(\hat{\nabla} \cdot \hat{\mathbf{u}}, \hat{w}) = (\hat{q}J, \hat{w}) \quad \text{for all } \hat{w} \in \hat{W}_h, \tag{21}$$

$$\langle \hat{\mathbf{u}} \cdot \hat{\nu}, \hat{\mu} \rangle_{\partial\hat{\Omega}_N} = \langle \hat{g}J_{\hat{\nu}}, \mu \rangle_{\partial\Omega_N} \quad \text{for all } \hat{\mu} \in \hat{\Lambda}_h, \tag{22}$$

where $\mathcal{K} = JDF^{-1}\mathbf{K}(DF^{-1})^T$. This is the discrete problem in $\hat{\Omega}$:

$$\hat{\mathbf{u}} = -\mathcal{K}\hat{\nabla}p, \quad \hat{\mathbf{x}} \in \hat{\Omega}, \tag{23}$$

$$\hat{\nabla} \cdot \hat{\mathbf{u}} = \hat{q}J, \quad \hat{\mathbf{x}} \in \hat{\Omega}, \tag{24}$$

$$\hat{p} = \hat{p}_0, \quad \hat{\mathbf{x}} \in \partial\hat{\Omega}_D, \tag{25}$$

$$\hat{\mathbf{u}} \cdot \hat{\nu} = \hat{g}J_{\hat{\nu}}, \quad \hat{\mathbf{x}} \in \partial\hat{\Omega}_N. \tag{26}$$

All computations are performed on the rectangular grid of $\hat{\Omega}$ after preprocessing the coefficients: $\mathbf{K}$ becomes $\mathcal{K}$, q becomes $\hat{q}J$, and g becomes $\hat{g}J_{\hat{\nu}}$.

The logically rectangular Cell-Centered Finite Difference Approximation.

To problem (19)–(22), we use the trapezoidal quadrature rule for approximating the three integrals involving a vector-vector product to obtain our cell-centered finite difference method on the logically rectangular mesh. As an illustration, consider a 2-D, uniform grid, with a constant $\mathcal{K}$. Denote the grid points and cell centers by

$$(\hat{x}_{i+1/2}, \hat{y}_{j+1/2}) \quad \text{and} \quad (\hat{x}_i, \hat{y}_j).$$

Then $\hat{\tilde{\mathbf{u}}} = -\hat{\nabla}\hat{p}$ is

$$\hat{\tilde{u}}^{\hat{x}}_{i+1/2,j} = -\frac{\hat{p}_{i+1,j} - \hat{p}_{i,j}}{\hat{h}}, \qquad \hat{\tilde{u}}^{\hat{y}}_{i,j+1/2} = -\frac{\hat{p}_{i,j+1} - \hat{p}_{i,j}}{\hat{h}}, \tag{27}$$

and $\hat{\mathbf{u}} = \mathcal{K}\hat{\tilde{\mathbf{u}}}$ is

$$\hat{u}^{\hat{x}}_{i+1/2,j} = \mathcal{K}_{11}\hat{\tilde{u}}^{\hat{x}}_{i+1/2,j} + \frac{\mathcal{K}_{12}}{4}\{\hat{\tilde{u}}^{\hat{y}}_{i+1,j-1/2} + \hat{\tilde{u}}^{\hat{y}}_{i+1,j+1/2} + \hat{\tilde{u}}^{\hat{y}}_{i,j-1/2} + \hat{\tilde{u}}^{\hat{y}}_{i,j+1/2}\}, \tag{28}$$

with a similar expression for $\hat{u}^{\hat{x}}_{i,j+1/2}$. Finally, for each element E_{ij}, $\hat{\nabla}\cdot\hat{\mathbf{u}} = \hat{q}J$ is

$$\left[\frac{\hat{u}^{\hat{x}}_{i+1/2,j} - \hat{u}^{\hat{x}}_{i-1/2,j}}{\hat{h}} + \frac{\hat{u}^{\hat{y}}_{i,j+1/2} - \hat{u}^{\hat{y}}_{i,j-1/2}}{\hat{h}}\right]\hat{h}^2 = \int_{\hat{E}_{ij}} \hat{q}J\, d\hat{x}. \tag{29}$$

The solution $\mathbf{u}$ on Ω is obtained from $p = \hat{p}$ and $\lambda = \hat{\lambda}$ using (16).

CONVERGENCE RESULTS

Let $\|\cdot\|$ denote the L^2-norm, $\|\varphi\|^2 = \int_\Omega |\varphi(\mathbf{x})|^2\, dx$, and let $|||\cdot|||_M$ denote the L^2-norm approximated by the midpoint quadrature rule. Before stating our result that the scheme is optimally convergent, we need the following definition.

Definition: An asymptotic family of grids is said to be generated by a C^2 map if each grid is an image by a fixed map of a grid that is uniform in each coordinate direction. Each component of the map must be strictly monotone and in $C^2(\bar{\Omega})$.

Theorem 1: There exists a constant C depending on the smoothness of F, $\mathbf{K}$, and the solution, but independent of the maximum grid spacing h, such that the cell-centered finite difference approximation satisfies

$$\begin{aligned}
&\|p_{\text{true}} - p_{\text{approx}}\| \le Ch,\\
&\|\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}}\| + \|\tilde{\mathbf{u}}_{\text{true}} - \tilde{\mathbf{u}}_{\text{approx}}\| \le Ch,\\
&\|\nabla\cdot(\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}})\| \le Ch.
\end{aligned}$$

Moreover,

$$\begin{aligned}
&|||p_{\text{true}} - p_{\text{approx}}|||_M \le Ch^2,\\
&|||\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}}|||_M + |||\tilde{\mathbf{u}}_{\text{true}} - \tilde{\mathbf{u}}_{\text{approx}}|||_M \le Ch^r,
\end{aligned}$$

where

$$r = \begin{cases} 2 & \text{if } K \text{ is diagonal and } \partial\Omega_N = \partial\Omega,\\ 3/2 & \text{if } K \text{ is diagonal or the grids are generated by a } C^2 \text{ map},\\ 1 & \text{otherwise.}\end{cases}$$

When K is diagonal or the grids are generated by a C^2 map, a half power of h is lost in the super-convergence result for the velocity. This is due strictly to effects near the boundary of the domain.

Theorem 2 (Interior estimates)*:* Let Ω' be compactly contained in Ω, and suppose that either K is diagonal or the grids are generated by a C^2 map. For any $\epsilon > 0$, there exists a constant C_ϵ depending on the smoothness of F, $\mathbf{K}$, and the solution, but independent of the maximum grid spacing h, such that

$$|||\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}}|||_{M,\Omega'} \leq C_\epsilon h^{2-\epsilon}.$$

The proofs of these results can be found in [6] (see also [23, 9]). These results are sharp in the sense that they are seen computationally in practical settings [9, 6].

DISCONTINUOUS MATERIAL PROPERTIES AND THE ENHANCED CELL-CENTERED FINITE DIFFERENCE METHOD

We show by example that our cell-centered scheme has difficulties approximating the solution when the material properties are discontinuous. On the unit square, let the true solution p and $\mathbf{K}$ be

$$p(x,y) = \begin{cases} xy & \text{for } x \leq 1/2, \\ xy + (x-1/2)(y+1/2) & \text{for } x > 1/2, \end{cases} \tag{30}$$

$$\mathbf{K}(x,y) = \begin{cases} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} & \text{for } x < 1/2, \\ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \text{for } x > 1/2. \end{cases} \tag{31}$$

Note that the eigenvectors for $\mathbf{K}$ are at 45 degrees to the grid for $x < 1/2$. Computationally, we see the following convergence rates:

$$|||p_{\text{true}} - p_{\text{approx}}|||_M \leq 0.06\, h^{0.96},$$
$$|||\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}}|||_M \leq 0.23\, h^{0.50}.$$

These are much worse that predicted by Theorem 1. The error is concentrated along the line $x = 1/2$.

If $\mathbf{K}$ or the map F is not smooth along an interface, then $\mathbf{u} = \mathbf{K}\mathbf{G}\check{\mathbf{u}}$ but not $\check{\mathbf{u}}$ is continuous in the normal direction. However, we have approximated $\check{\mathbf{u}}$ in the same space as $\mathbf{u}$, i.e., $\mathbf{V}_h$, which has continuous normal components. We must relax this continuity along any interface where the material properties change discontinuously. To do so for the approximation of $\check{\mathbf{u}}$ but not $\mathbf{u}$ would make the matrix A in (14) non-square and therefore not fully invertible. We therefore need to relax the continuity of $\mathbf{V}_h$ for both $\check{\mathbf{u}}$ and $\mathbf{u}$.

This idea originates in the hybrid form of the mixed method of Arnold and Brezzi [11]. Introduce Lagrange multiplier pressures living on the element edges or faces of the discontinuity interface Γ (we already have them on $\partial\Omega_N$), and add a condition that specifies that $\mathbf{u}$ alone is continuous across Γ. That is, replace (11) in (10)–(13) and add (33):

$$(\mathbf{G}\check{\mathbf{u}}, \mathbf{v}) - \sum_E (p, \nabla \cdot \mathbf{v})_E = -\langle p_0, \mathbf{v} \cdot \nu \rangle_{\partial\Omega_D} - \sum_E \langle \lambda, \mathbf{v} \cdot \nu \rangle_{\partial E \cap (\partial\Omega_N \cup \Gamma)} \quad \text{for all } \mathbf{v} \in \mathbf{V}_h, \tag{32}$$

$$\sum_E \langle \mathbf{u} \cdot \nu, \mu \rangle_{\partial E \cap \Gamma} = 0 \quad \text{for all } \mu \in \Lambda_h. \tag{33}$$

We call this scheme the enhanced cell-centered finite difference scheme. It can be formulated without explicit reference to Lagrange pressures by taking a mesh with zero width cells on Γ. The infinitely thin cell's pressure is the Lagrange pressure [22].

Using the enhanced method, the same computational example shows the following convergence rates:

$$|||p_{\text{true}} - p_{\text{approx}}|||_M \leq 0.18\, h^{2.02},$$
$$|||\mathbf{u}_{\text{true}} - \mathbf{u}_{\text{approx}}|||_M \leq 0.10\, h^{1.49}.$$

The Hybrid Form of the Mixed Method.

It should be noted that the hybrid form of the mixed method uses Lagrange multiplier pressures along all faces. By eliminating all but the Lagrange pressures leads to a Shur complement system that is sparse, symmetric, and positive definite. Unfortunately, there are more unknowns than the number of elements. In 2-D, if deformed rectangles are used, there are two times as many unknowns. In 3-D, deformed brick elements need three times as many unknowns.

TWO-PHASE FLOW

We consider the accuracy of mixed finite element methods for approximating the highly nonlinear problem of two-phase flow of incompressible water and air (or oil or a NAPL). This represents work of two of the authors and Nai-Ying Zhang [10]. The governing equations are

$$\phi \frac{\partial s}{\partial t} - \nabla \cdot [K \lambda_w(s) \nabla p_w] = q_w(s), \tag{34}$$
$$-\phi \frac{\partial s}{\partial t} - \nabla \cdot [K \lambda_a(s) \nabla p_a] = q_a(s), \tag{35}$$
$$p_c(s) = p_a - p_w, \tag{36}$$

where $0 \leq s(\mathbf{x}, t) \leq 1$ is the (normalized) wetting fluid saturation, ϕ is the porosity, $\lambda_\alpha = k_{r\alpha}(s)/\mu_\alpha$ is the relative mobility of phase $\alpha = w, a$, and p_c is the capillary pressure.

Define total velocity

$$\mathbf{v} = -K \lambda_w \nabla p_w - K \lambda_a \nabla p_a. \tag{37}$$

By rearranging (34)–(35) and using (36), we can obtain the pressure equation

$$\nabla \cdot \mathbf{v} = -\nabla \cdot (K(\lambda_w + \lambda_a) \nabla p_w + K \lambda_a \nabla p_c) = q_w + q_a \tag{38}$$

and the saturation equation

$$\phi \frac{\partial s}{\partial t} + \nabla \cdot \left(K \frac{\lambda_w \lambda_a}{\lambda_w + \lambda_a} \nabla p_c + \frac{\lambda_w}{\lambda_w + \lambda_a} \mathbf{v} \right) = q_w. \tag{39}$$

The pressure equation is a well behaved elliptic equation; however, the saturation equation is degenerate parabolic, so concentrate on it.

Kirchhoff Transformation.

Define the Kirchhoff Transformation

$$P(s) = -\int_0^s \left(\frac{\lambda_w \lambda_a}{\lambda_w + \lambda_a} p_c'\right)(\sigma)\, d\sigma. \tag{40}$$

Then $\nabla P(s) = -\dfrac{\lambda_w \lambda_a}{\lambda_w + \lambda_a} \nabla p_c$, and the saturation equation takes the form

$$\phi \frac{\partial s}{\partial t} - \nabla \cdot [\alpha \nabla P(s) + \beta(P(s))] = \gamma(P(s)). \tag{41}$$

Regularity (Smoothness) of the Solution.

We assume that $P(s)$ is strictly monotone increasing, that $P'(s)$ may be zero (degenerate parabolic), but there is a constant $C_0 > 0$ such that

$$\|P(\varphi_1) - P(\varphi_2)\|^2 \le C_0 (P(\varphi_1) - P(\varphi_2), \varphi_1 - \varphi_2).$$

We also assume that β and γ are Lipschitz continuous. These assumptions can be justified on physical grounds [10, 3].

Introduce a new variable

$$\psi = -\alpha \nabla P(s) - \beta(P(s)). \tag{42}$$

It is known [2, 1, 3] that s is continuous and

$$s \in L^\infty(L^\infty), \quad \frac{\partial s}{\partial t} \in L^2(H^{-1}), \quad \psi \in L^2((L^2)^d), \quad \gamma(P(s)) \in L^2(L^2),$$

where H^{-1} is the dual of H_0^1 and the outer function space refers to the time interval of interest and the inner one to Ω. The low regularity is due to the degenerate diffusion. As we pass from a strictly two-phase region to a region with a single phase, the solution is not particularly smooth; thus, it is very difficult to approximate the solution accurately.

Many authors have considered the approximation properties of the continuous, piecewise linear finite element Galerkin method. However, cell-centered finite difference methods are commonly used to solve this problem [18]. Since the mixed finite element method is strongly related to cell-centered finite difference methods, we present a mixed method analysis. Such an analysis has not previously appeared. Our approach is to consider the problem from the point of view of optimal approximation; that is, can we approximate the solution as well as possible, given the finite element approximating space. Since typically the interfaces between the single and two-phase regions occupy a fairly small part of the domain, we can then expect to have very good approximation of the solution.

A NONLINEAR MIXED METHOD

In a standard mixed variational form for (41),

$$\left(\phi \frac{\partial s}{\partial t}, w\right) + (\nabla \cdot \psi, w) = (\gamma(P(s)), w) \quad \text{for all } w \in H_0^1. \tag{43}$$

Since we can only expect in general that $\partial s/\partial t \in L^2(H^{-1})$, the trial functions must belong to $H_0^1(\Omega)$. To avoid this, following Nochetto [17], we integrate (41) in time to obtain

$$s(\mathbf{x},t) + \nabla \cdot \int_0^t \psi \, d\tau = \int_0^t \gamma(P(s)) \, d\tau + s_0(\mathbf{x}),$$

where s_0 is the initial saturation. Note that

$$\int_0^t \psi \, d\tau \in H^1((L^2)^d) \cap L^2(H(\mathrm{div})),$$

so we can formulate a mixed variational form as

$$(s(\cdot,t), w) + \Big(\nabla \cdot \int_0^t \psi \, d\tau, w\Big) = \Big(\int_0^t \gamma(P(s)) \, d\tau, w\Big) + (s_0, w) \quad \text{for all } w \in L^2, \tag{44}$$

$$(\alpha^{-1}[\psi + \beta(P(s))], \mathbf{v}) - (P(s), \nabla \cdot \mathbf{v}) = -\langle P(s_D), \mathbf{v} \cdot \nu \rangle \quad \text{for all } \mathbf{v} \in H(\mathrm{div}), \tag{45}$$

where s_D is, say, a Dirichlet boundary condition.

Now let Ω be partitioned into a conforming finite element mesh with maximal element diameter h. Let $W_h \times \mathbf{V}_h \subset L^2 \times H(\mathrm{div})$ be any standard mixed finite element space. Let $\Delta t > 0$, $t_n = n\Delta t$, and $\varphi^n = \varphi(t_n)$.

Our nonlinear mixed method is to find $s^n \approx S^n \in W_h$ and $\psi^n \approx \Psi^n \in \mathbf{V}_h$ satisfying

$$(S^n, w) + \Big(\nabla \cdot \sum_{j=1}^n \Psi^j \, \Delta t, w\Big) = \Big(\sum_{j=1}^n \gamma(P(S^j)) \, \Delta t, w\Big) + (s_0, w) \quad \text{for all } w \in W_h, \tag{46}$$

$$(\alpha^{-1}[\Psi^n + \beta(P(S^n))], \mathbf{v}) - (P(S^n), \nabla \cdot \mathbf{v}) = -\langle P(s_D^n), \mathbf{v} \cdot \nu \rangle \quad \text{for all } \mathbf{v} \in \mathbf{V}_h. \tag{47}$$

The first equation is equivalent to the usual backward Euler form

$$\Big(\frac{S^n - S^{n-1}}{\Delta t}, w\Big) + (\nabla \cdot \Psi^n, w) = (\gamma(P(S^n)), w) \quad \text{for all } w \in W_h, \tag{48}$$

$$(S^0, w) = (s_0, w) \quad \text{for all } w \in W_h. \tag{49}$$

Let $\mathcal{P}_{W_h}$ and $\mathcal{P}_{V_h}$ denote L^2-projection into W_h and $\mathbf{V}_h$, respectively. Let Π denote the usual element based flux-preserving projection operator for mixed methods [19, 12]. Such projections are optimal in their approximation properties.

Theorem 3: For the nonlinear mixed finite element approximation,

$$\begin{aligned}
&\sum_{j=1}^n (S^j - s^j, P(S^j) - P(s^j)) \, \Delta t + \Big\| \sum_{j=1}^n \Psi^j \, \Delta t - \mathcal{P}_{V_h} \int_0^{t_n} \psi \, d\tau \Big\|^2 \\
&\quad \le C \sum_{j=1}^n \Big\{ \|\mathcal{P}_{W_h} s^j - s^j\|^2 + \Big\|(\mathcal{P}_{V_h} - I) \int_0^{t_j} \psi \, d\tau \Big\|^2 + \Big\|\nabla \cdot (\Pi - \mathcal{P}_{V_h}) \int_0^{t_j} \psi \, d\tau \Big\|^2 \\
&\qquad + \Big\| \sum_{i=1}^j \gamma(P(s^i)) \, \Delta t - \int_0^{t_j} \gamma(P(s)) \, d\tau \Big\|^2 + \Big\| \frac{1}{\Delta t} \int_{t_{j-1}}^{t_j} \psi \, d\tau - \psi^j \Big\|^2 \Big\} \Delta t,
\end{aligned}$$

and

$$\begin{aligned}
\|S^n - s^n\|_{H^{-1}} \le C \Big\{ & h \|\mathcal{P}_{W_h} s^n - s^n\| + \Big\| \sum_{j=1}^n \Psi^j \, \Delta t - \Pi \int_0^{t_n} \psi \, d\tau \Big\| \\
& + \sum_{j=1}^n \|P(S^j) - P(s^j)\| \, \Delta t + \Big\| \sum_{j=1}^n \gamma(P(s^j)) \, \Delta t - \int_0^{t_n} \gamma(P(s)) \, d\tau \Big\|^2 \Big\}.
\end{aligned}$$

The form $\left\{ \int_0^t (S-s, P(S)-P(s))\, d\tau \right\}^{1/2}$ bounds the size of $S-s$; for example, it bounds the norm $\|P(S)-P(s)\|$. It is *not*, however, a norm itself. It may even fail to be a metric. Also, $\|\cdot\|_{H^{-1}} = \sup_{\varphi \in H_0^1} (\cdot, \varphi)/\|\varphi\|_{H^1}$. The theorem says that the saturation, in a weak H^{-1}-norm sense, is bounded by optimal approximation terms, time truncation terms, and a term involving the divergence that is essentially optimal in character.

CONCLUSIONS

We have developed a cell-centered finite difference mixed method as an approximation to an expanded mixed finite element method. It is suitable for groundwater flow and transport problems on general geometry with tensor permeabilities or dispersivities. It is both locally (element-by-element) mass conservative and highly accurate.

General geometry can be handled by a mapping between the computational and physical domains. The coefficients are transformed in a simple way before commencing the computation. On a logically rectangular mesh, special quadrature rules are applied to the expanded finite element method to transform it into a cell-centered finite difference method with a stencil of 9 points in 2-D and 19 points in 3-D, allowing easy and efficient implementation. Similar results hold for triangular meshes [4, 5, 6].

The solution of the logically rectangular cell-centered finite difference scheme converges to the true solution at the optimal order as the mesh is refined; moreover, superconvergence is attained by the velocity at certain discrete points of the domain on C^2-smooth grids away from the boundary. We saw that grid geometry strongly affects the approximation error, so it is necessary to define and refine grids in a C^2-smooth manner.

Lagrange multiplier pressures or infinitely thin cells need to be introduced along faces where the tensor or geometry changes discontinuously. This allows the adjusted pressure gradient $\tilde{\mathbf{u}}$ to be discontinuous, so that the coefficient times $\tilde{\mathbf{u}}$ approximates well the continuous velocity $\mathbf{u}$.

Mixed methods accurately approximate two-phase flow. The Kirchoff transformation may be useful in computations. The interface between single and two-phase regions is captured in an approximate (H^{-1}-norm) sense.

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