Computation of variably saturated subsurface flow by adaptive mixed hybrid finite element methods

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Received 24 December 2002; received in revised form 28 October 2003; accepted 19 March 2004

Abstract

We present adaptive mixed hybrid finite element discretizations of the Richards equation, a nonlinear parabolic partial differential equation modeling the flow of water into a variably saturated porous medium. The approach simultaneously constructs approximations of the flux and the pressure head in Raviart–Thomas spaces. The resulting nonlinear systems of equations are solved by a Newton method. For the linear problems of the Newton iteration a multigrid algorithm is used. We consider two different kinds of error indicators for space adaptive grid refinement: superconvergence and residual based indicators. They can be calculated easily by means of the available finite element approximations. This seems attractive for computations since no additional (sub-)problems have to be solved. Computational experiments conducted for realistic water table recharge problems illustrate the effectiveness and robustness of the approach.

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Keywords: Saturated–unsaturated flow; Nonlinear elliptic–parabolic problem; Mixed finite element method; Raviart–Thomas spaces; A posteriori error indicator

1. Introduction

Accurate, reliable and efficient simulations of moisture fluxes through porous media are desirable in hydrological and environmental studies, as well as in civil and environmental engineering. The ability to model time dependent flows in composite soil formations that may be intermittently saturated and drained is particularly important from the point of view of physical realism. This paper focuses on an appropriate and controlled treatment of saturated–unsaturated subsurface flows, ensuring accuracy and efficiency in a robust space adaptive grid refinement algorithm.

Numerous papers have been written on numerical schemes for the Richards equation which is typically used to describe variably saturated flow in porous media. The most successful approximation schemes have been based on conservative methods; cf. [18,33]. In this work we present an adaptive mixed finite element discretization scheme of the Richards equation. Mixed finite element methods have become popular in recent years for modeling flow in porous media due to their inherent conservation properties and the fact that the models provide flux approximations as part of the formulation. These fluxes are often of greater importance than the pressure head itself. We will consider a hybrid variant of the mixed finite element method with lowest order Raviart–Thomas spaces by applying the Lagrange multiplier technique (cf., e.g., [16]) to the nonlinear and possibly degenerate Richards equation. The Lagrange multipliers then become the unknowns of a global nonlinear system of equations which we solve by a damped version of Newton’s method combined with a W-cycle multigrid algorithm for the linear problems of the Newton iteration. For linear elliptic problems it is well known that the Lagrange multiplier approach provides certain implementational advantages over the standard mixed formulation of the problem, for instance, for building the multigrid algorithm (cf. [21]) and an adaptive grid refinement algorithm by superconvergence based a posteriori error estimation (cf. [43]). As we shall see, these advantages can be carried over to the Richards equation. However, since this one is nonlinear,
the discrete equation of continuity does not allow an explicit representation of the piecewise constant pressure approximation in terms of the Lagrange multipliers and, thereby, an elimination of the pressure variable. This complicates the application of the multiplier technique. It has rather to be embedded into the Newton iteration by computing after each Newton correction of the Lagrange multipliers the pressure values in terms of elementwise nonlinear problems which we again solve by Newton’s method. In the subsequent Newton step the Jacobian matrix is then calculated in terms of these recomputed pressure values. The flux approximation is determined locally by some postprocessing procedure. The convergence of the scheme will be demonstrated by numerical experiments. For analyses of the mixed approach to the Richards equation we refer to [3,36,44].

Our principal objective, which is certainly a long range one, is to develop robust efficient and mathematically rigorous adaptive (finite element) approximation schemes for the Richards equation of variably saturated subsurface flow by, firstly, establishing existence and regularity, then, based on these results, proving efficient and reliable sharp a posteriori error estimates for a space–time adaptive algorithm and, finally, providing convergence proofs for the (non-)linear solver. However, our current approach still relies, in the general nonlinear and degenerate case, on heuristic arguments which are either physically reasonable or confirmed by our computations. For saturated flow all arguments are rigorous and based on proofs. In scientific computing, techniques which were developed and emerged to work well for simple (linear) problems are naturally applied to more general and sophisticated ones. This is also done here by considering variably saturated flow as a perturbation of saturated flow.

In this work we present an adaptive variant of the mixed finite element approach to the Richards equation by applying a posteriori error estimators established for linear elliptic problems (cf. [43]) to our degenerate nonlinear one. This leads to error indicators in contrast to sharp error estimators verified by a rigorous mathematical analysis. The resulting error indicators are rather easy and fast to evaluate by means of the already computed finite element approximations and yield convincing numerical results. First, a superconvergence based error indicator for the pressure head is proposed which is due to some specific superconvergence approximation property of the mixed hybrid finite element method (cf. [16]). Then, this concept is carried over to the flux variable. By a simple post processing of its tangential components on interelement edges (cf. [11]) an additional higher order approximation of the flux is obtained which directly gives rise to an error indicator. Finally, a residual based error indicator for the total error of pressure head and flux is presented which relies on a Helmholtz decomposition of the flux ansatz space; cf. [17,43]. In calculations our adaptive grid refinement algorithm nicely resolves steep saturation fronts with high accuracy, that occur as water infiltrates dry soil, and leads to smaller discretization errors than an uniform triangulation; cf. Section 8.

Alternative adaptive approaches to subsurface flow and related problems are described, e.g., in [22,23,28,40]. In [40], a least-squares mixed finite element method is introduced for the Richards equation with refinement strategies based on local least-squares functionals. In [23], a Zienkiewicz and Zhu type error indicator [45] is designed for multiphase problems. In [28], a moving mesh technique is proposed. In [22], mixed and Galerkin methods are combined and iterative techniques of domain decomposition type are used.

The plan for the paper is as follows. First, we introduce the Richards equation of variably saturated subsurface flow, recall regularity results and give basic notations. In Section 3 its mixed hybrid finite element approximation is briefly presented; cf. also [19]. Section 4 is devoted to the solution process of the resulting nonlinear algebraic system of equations. The elimination of internal degrees of freedom and the (non-)linear solver are described. In Section 5, the theoretical convergence rates of the linear elliptic case (cf. [16]) are verified for two one-dimensional nonlinear degenerate problems. In Section 6 we present two-dimensional numerical tests with steep fronts. Section 7 is devoted to the adaptive techniques. The error indicators for the mixed hybrid finite element approximation of the Richards equation are given and our adaptive mesh refinement algorithm is described. In Section 8 numerical tests are presented. One of the water table recharge problems is recomputed by the proposed adaptive method. Additionally, it is shown for one test case that the adaptive grid refinement in fact leads to smaller errors than the uniform triangulation. We end with conclusions.

2. Formulation of the problem

We consider saturated–unsaturated flow in soil modeled by the Richards equation

$$\partial_t \Theta(\psi) - \nabla \cdot (K(\psi) \nabla (\psi + z)) = f$$  \hspace{1cm} (1)$$

for the pressure head $\psi : \Omega \to \mathbb{R}$ in a polyhedral domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or $3$, with boundary $\Gamma$. The pore spaces may contain both water and air. The “saturated zone” is the portion of the medium that is water saturated, while the “unsaturated zone” contains both water and air. These zones may vary with space and time. In (1), $\Theta(\psi)$ denotes the volumetric water content and $K(\psi) = K_s k_{rw}(\Theta(\psi))$ denotes the permeability where $K_s = k_s \mu / \rho$ and $k_{rw}$ is the

\[
\frac{\text{at} \partial \Theta(\psi) - \nabla \cdot (K(\psi) \nabla (\psi + z)) = f}{\text{for the pressure head } \psi : \Omega \to \mathbb{R} \text{ in a polyhedral domain } \Omega \subset \mathbb{R}^d, \text{ with boundary } \Gamma. \text{ The pore spaces may contain both water and air. The “saturated zone” is the portion of the medium that is water saturated, while the “unsaturated zone” contains both water and air. These zones may vary with space and time. In (1), } \Theta(\psi) \text{ denotes the volumetric water content and } K(\psi) = K_s k_{rw}(\Theta(\psi)) \text{ denotes the permeability where } K_s = k_s \mu / \rho. \text{ And } k_{rw} \text{ is the permeability in the saturated zone.} \]
relative permeability of water to air in the unsaturated regime. The constant $k_s$ is the absolute permeability, $\rho$ is the water density, $g$ is the gravitational acceleration constant and $\mu$ is the water viscosity. The function $f$ describes sources and sinks. The hydraulic head $\psi + z$ represents the height of the water column above some reference elevation ($z = 0$). The elevation $z$ at any point is simply the height of that point (against the gravitational direction), and the pressure head indicates the vertical distance between the point and the water table. Functional forms for $\Theta(\psi)$ and $K(\psi)$, both of which are bounded, have been derived in the literature. In our computations we use models based on [26,34,35]. The relations given in [26,34] lead to unbounded $K'(\psi)$ in the neighborhood of the saturated limit for some types of soil. This is avoided by a suitable modification of $K(\psi)$ close to the saturated regime; cf. Section 6.

The formulation of Richards equation given above assumes that the medium itself is incompressible and thus that the porosity $\phi$ does not change with time or hydraulic head. The formulation is valid for the two regimes of our interest. Where the medium is fully water saturated, $\Theta(\psi) = \phi$ and $k_{sw}(\Theta(\psi)) = 1$. Where the medium is partially water saturated, $\Theta'(\psi) > 0$ and $0 < k_{sw} < 1$. Thus, (1) is elliptic in the saturated zone and parabolic in the unsaturated zone. Moreover, both regimes can exist within a single flow domain. In this paper we do not consider dry regions where the medium is (nearly) air saturated and $K(\psi)$, as well as $K'(\psi)$ and $\Theta'(\psi)$, may be very small. In this case, Eq. (1) effectively reduces to the system (cf. (4) and (5) below)

$$\nabla \cdot q = f, \quad q = 0,$$

for the flux $q$, leaving $\psi$ completely undetermined. Dry regions are beyond the scope of our applications. However, in such case one may regularize (1) by replacing $K(\psi)$ with $\tilde{K}(\psi) = K_{min} + (1 - K_{min}/K_s)K(\psi)$ and $K_{min} \leq K_s$ which implies that $0 < K_{min} \leq \tilde{K}(\psi) \leq K_s$ uniformly in $\Omega$; cf. [40]. Of course, one needs to be very careful with the choice of $K_{min}$ to make sure that the computational results are still meaningful. A numerical sensitivity study may be helpful for an appropriate choice of the parameter $K_{min}$.

Let $\Gamma_D$ be the portion of the boundary $\partial \Omega$ of $\Omega$ where Dirichlet conditions are specified, and let $\Gamma_N$ be the portion where Neumann conditions are specified. We assume that $\partial \Omega = \Gamma_D \cup \Gamma_N$. We consider solving Richards equation (1) over $J \times \Omega$, where $J = (0, T)$ and $T > 0$ is some final time. Boundary and initial conditions are given as

$$\psi = g_D \quad \text{on} \quad \Gamma_D,$$

$$-K(\psi)\nabla(\psi + z) \cdot n = g_N \quad \text{on} \quad \Gamma_N,$$

$$\psi = \psi_0 \quad \text{for} \quad t = 0.$$

Here, $\psi$ denotes the outer unit normal to $\partial \Omega$. Only in order to simplify the notation, we tacitly assume from now on that $g_N = 0$ and $f = 0$.

Then, Eq. (1) can be rewritten as the following equivalent system of equations:

$$\partial_t \Theta(\psi) + \nabla \cdot q = 0, \quad (4)$$
$$q + K(\psi)\nabla(\psi + z) = 0. \quad (5)$$

Eq. (4) describes the conservation of mass. Eq. (5) which links the flux $q$ to the hydraulic head is the Darcy law; cf., e.g., [8]. Alt and Luckhaus [2] state the following existence and regularity result for the system (4) and (5):

$$\Theta(\psi) \in L^\infty(J; L^1(\Omega)), \quad q \in L^2(J; L^2(\Omega)),$$
$$\partial_t \Theta(\psi) \in L^2(J; W^{-1}_2(\Omega)). \quad (6)$$

Here, $L^p(\Omega)$ and $W^k_p(\Omega)$ are the standard Lebesgue and Sobolev spaces; cf., e.g., [1]. By $W^{-1}_2(\Omega)$, for $k$ a positive integer, we denote the dual space of $W^k_2(\Omega)$. For $p \in [1, \infty]$ and a Banach space $X$ we denote by $L^p(J; X)$ the space of strongly measurable functions $u : J \to X$ such that $\left( \int_J \| u(t) \|_X^p \, dt \right)^{1/p} < \infty$ if $1 \leq p < \infty$ and $\text{ess sup}_J \| u(t) \|_X < \infty$ if $p = \infty$. We do not distinguish through the notation between scalar and vector valued functions, or function spaces, or norms. The precise meaning is always clear from the context. By $\langle \cdot, \cdot \rangle$ we will denote the $L^2(\Omega)$ inner product, and $\| \cdot \|$ is its norm.

According to (6), $\partial_t \Theta(\psi) \in L^2(J; W^{-1}_2(\Omega))$ can generally be assumed only. Hence, a variational formulation of (4) relying on (6) would require test functions for (4) to be taken in $W^1_2(\Omega)$. In order to relax this requirement, an alternate time integrated variational formulation based on the Kirchhoff transformation, a term which requires computing integrals of the permeability, may be used for the approximation of the system (4), (5). For details of this technique and an error analysis for the finite element approximation of the time integrated problem we refer to [3,36,44]. Our discretization and computations are based on the untransformed formulation (4), (5). This saves compute time since there is no need for integrated values of the transformation. The test problems in Sections 6 and 8 will show that our approach leads to robust and stable approximations of the Richards equation also in degenerate cases.

The regularity result (6) does not ensure that $\Theta(\psi)$ exists pointwise everywhere in time. However, we know that since $\Theta(\psi)$ physically represents water saturation, $\Theta(\psi)$ is defined pointwise at every time. Thus we may assume that

$$\Theta(\psi) \in L^\infty(J; L^\infty(\Omega))$$

such that, below, test functions for the time discrete version of Eq. (4) may be chosen in $L^2(\Omega)$ instead of $W^1_2(\Omega)$. We further assume that

$$\Theta(\psi) \in L^\infty(J; L^\infty(\Omega))$$
3. Mixed finite element discretization

Let $\Pi_h = \{K\}$ be a finite element decomposition of mesh size $h$ of the polyhedral domain $\mathcal{D}$ into closed subsets $K$, triangles in two dimensions and tetrahedrons in three dimensions. The decompositions are assumed to be face to face. The set of faces is denoted by $\partial_h = \partial_h^1 \cup \partial_h^D \cup \partial_h^N$ where $\partial_h^1$ refers to the interior faces and $\partial_h^D$ and $\partial_h^N$ to those located on $\Gamma_D$ and $\Gamma_N$, respectively. We use the notation “face” in the two- and three-dimensional case. If $d = 2$, then the faces are the sides of the triangles. We form discrete subspaces of $W_h$ and $V_h$ of $L^2(\Omega)$ and $H_{0,N}(\Omega;\text{div})$ using the lowest order mixed finite element spaces of Raviart–Thomas; cf., e.g., [16].

Restricting our approach to the lowest order Raviart–Thomas spaces does not seem to be strongly limiting since the solution most likely lacks enough regularity needed for getting a global improvement by using higher order finite elements. Nevertheless, for the future we plan to test higher order mixed finite elements, e.g., $RT_l$ or $BDM_l$ elements; cf. [16]. We expect a local improvement by such elements, for instance, inside the saturated or unsaturated zones, respectively, since the solution may admit higher regularity there.

In what follows let

$$ W_h = \{w_h \in W; w_h|K \in P_0(K) \quad \forall K\}, $$

$$ V_h = \{v_h \in V; v_h|K \in RT_0(K) \quad \forall K\} $$

denote the lowest order Raviart–Thomas spaces (cf., e.g., [16]) where $RT_0(K) = P_0(K)^d + xP_0(K)$ with $P_0(K)$ denoting the set of all polynomials on $K$ of degree less or equal than 1 and $x = (x_1, \ldots, x_d), x \in K$. A fully discrete mixed approximation $(\psi^{n, a}_h, q^{n, a}_h)$ of (1)–(3) is now obtained by solving (7) in $W_h \times V_h$. In what follows, we tacitly assume that $(\psi^{n, a}_h, q^{n, a}_h)$ exists uniquely.

From the linear elliptic case, which corresponds to the saturated regime, it is known that the discrete version of (7) leads to a linear system of equations with an indefinite matrix; cf. [16, p. 178]. This is definitely a considerable source of trouble for solving the linear system. To overcome this difficulty, we use the technique of interelement Lagrange multipliers (cf., e.g., [16]) which can also be interpreted as a hybridization of the mixed formulation (7). In the elliptic case this approach leads to a linear system of equations with a positive definite matrix. Hence, standard linear solvers can be used for solving the system. The degenerate nonlinear case is more complex. However, the technique of interelement multipliers can also be applied to this case. For an analysis of the technique in more general cases than the linear we refer to [19] as well as [4, 14, 15].

The condition $v \in H(\Omega; \text{div})$ implies the continuity of the normal component of the fluxes over interior faces; cf. [7]. The basic idea of interelement Lagrange multipliers consists in first weakening and then reformulating the continuity constraint for the normal component of the fluxes over interelement boundaries. By weakening the continuity constraint we enlarge the approximation space $V_h$. This enables us to eliminate internal degrees of freedom which is better known as static condensation. The enlarged approximation space for the flux variable is defined by

$$ \hat{V}_h = \{v_h \in L^2(\Omega); v_h|K \in RT_0(K) \quad \forall K\}. $$

The condition $v_h \in \hat{V}_h$ does not necessarily imply the continuity of the normal component of the fluxes over interior faces. For the Lagrange multipliers we introduce the function space

$$ M_{h, g} = \left\{ \mu_h \in L^2(\partial_h^D); \mu_h|E \in P_0(E) \quad \forall E \in \partial_h^D, \right\} $$

and $M_{h, 0} = M_{h, g}$. If $v_h \in \hat{V}_h$, then (cf. [16, p. 179])

$$ \sum_{K \in \Pi_h} \langle v_h \cdot n, \mu_h \rangle_{\partial K} = 0 \quad \text{for all } \mu_h \in M_0 \text{ if and only if } v_h \in V_h. $$

This implies the following mixed hybrid finite element approximation of (1)–(3):

For given $(\psi^{n, a}_h, q^{n, a}_h)$, find $(\psi^{n, a}_h, q^{n, a}_h, z_h) \in W_h \times \hat{V}_h \times M_{h, g}$ such that there holds

$$ q \in L^\infty(J; H(\Omega; \text{div})), $$

where $H(\Omega; \text{div}) = \{q \in L^2(\Omega) | \nabla \cdot q \in L^2(\Omega) \}$. We also need the subspace $H_{0,N}(\Omega; \text{div}) = \{q \in H(\Omega; \text{div}) | (\nabla \cdot q, w)_{\Omega_1} = 0 \quad \forall w \in H^1_D(\Omega) \}$ where $H^1_D(\Omega) = \{w \in W^1_2(\Omega) \mid (\nabla w|_{\Gamma_D}, \nu) = 0 \}$. Here, $(\cdot, \cdot)_{\Omega_1}$ denotes the duality between $H^{-1/2}(\Omega)$ and $H^{1/2}(\Omega)$; cf. [16] for details. For short, we set $W = L^2(\Omega)$ and $V = H_{0,N}(\Omega; \text{div})$. Now we discretize the Eqs. (4) and (5) in time by an implicit Euler scheme. This gives rise to the following mixed variational problem:

For given $\psi^{n-1} \in W$ find $(\psi^n, q^n) \in W \times V$ such that there holds

$$ \langle \Theta(\psi^n), w \rangle + \tau_n (\nabla \cdot q^n, w) = \langle \Theta(\psi^{n-1}), w \rangle, $$

$$ \langle K(\psi^n)^{-1} q^n, v \rangle - \langle \psi^n, \nabla \cdot v \rangle + \langle \nabla z, v \rangle = -\langle g_D^n, v \cdot \nu \rangle_{\Gamma_D} $$

(7)

for all $w \in W, v \in V$ and $n \geq 1$.

Here, $\tau_n = t_n - t_{n-1}$ is the time step size and $g_D^n = g_D(t_n, \cdot)$. The starting value is $\psi^0 = \psi_0$. Since we do not consider the case of a fully dry porous medium with vanishing $K$ in this paper, the term $K(\psi^n)^{-1}$ in (7) is well defined. In practical computations one may bound $K$ from below by $\kappa K$ with some sufficiently small factor $\kappa$. The variational problem (7) represents the dual mixed variational problem:

In the two- and three-dimensional mixed variational problem:

the notation “face” in the two- and three-dimensional case. If $d = 2$, then the faces are the sides of the triangles. We form discrete subspaces of $W_h$ and $V_h$ of $L^2(\Omega)$ and $H_{0,N}(\Omega; \text{div})$ using the lowest order mixed finite element spaces of Raviart–Thomas; cf., e.g., [16].

Restricting our approach to the lowest order Raviart–Thomas spaces does not seem to be strongly limiting since the solution most likely lacks enough regularity needed for getting a global improvement by using higher order finite elements. Nevertheless, for the future we plan to test higher order mixed finite elements, e.g., $RT_l$ or $BDM_l$ elements; cf. [16]. We expect a local improvement by such elements, for instance, inside the saturated or unsaturated zones, respectively, since the solution may admit higher regularity there.
\[
\langle \psi_h^n, w_h \rangle + \tau_n \langle \nabla_h \cdot q_h^n, w_h \rangle = \langle \Theta(\psi_h^{n-1}), w_h \rangle,
\]

\[
\langle K(\psi_h^{n-1})^{-1} q_h^n, v_h \rangle - \langle \psi_h^{n-1}, \nabla_h \cdot v_h \rangle + \langle \nabla z, v_h \rangle
\]

\[
= - \sum_{K \in \mathcal{H}_h} \langle \lambda_h^n, v_h \cdot v \rangle_{\mathcal{E}K},
\]

\[
\sum_{K \in \mathcal{H}_h} \langle q_h^n \cdot v, \mu_h \rangle_{\mathcal{E}K} = 0
\]

for all \(w_h \in W_h, v_h \in \tilde{V}_h, \mu_h \in M_h\) and \(n \geq 1\).

In (8), the operator \(\nabla_h^n\) denotes the gradient operator understood in the piecewise sense with respect to the decomposition \(\Pi_h\), rather than in the distributional sense with respect to \(\Omega\). In particular, \(q_h^n \in V_h\) is ensured. For nonhomogeneous Neumann boundary conditions \(g_N \neq 0\), we get \(\sum_{K \in \mathcal{H}_h} \langle q_h^n \cdot v, \mu_h \rangle_{\mathcal{E}K} = \langle g_N, \mu_h \rangle_{\Gamma_N}\) for all \(\mu_h \in M_h\) instead of the last of the identities (8).

4. Elimination of internal degrees of freedom and solution algorithm

The mixed hybrid finite element approximation (8) looks even more complex than the original formulation (7). But now we can eliminate the internal degrees of freedom of the system (8). In the following we shall eliminate the flux variable \(q_h^n\) and the pressure function \(\psi_h^n\). Then the interelement Lagrange multipliers \(\lambda_h^n\) become the unknowns of a global nonlinear system of equations which we solve by a Newton method and a multigrid algorithm. Finally, the flux \(q_h^n\) and the pressure \(\psi_h^n\) can be recovered locally, that is, elementwise, from the Lagrange multipliers by some post processing procedure. We describe the elimination of the internal degrees of freedom for the two-dimensional case \(d = 2\) only. The techniques can be applied analogously for \(d = 3\). However, the computations become more complex.

To eliminate the flux variable \(q_h^n\) and the pressure function \(\psi_h^n\), we first rewrite (8) as an algebraic system of equations. In terms of basis functions, the solution \((\psi_h^n, q_h^n, \lambda_h^n) \in W_h \times V_h \times M_h\) of the system (8) admits the representation

\[
\psi_h^n = \sum_{K \in \mathcal{H}_h} \psi_h^n_{X,K}, \quad q_h^n = \sum_{E \in \mathcal{E}h} q_E^n w_E
\]

and, similarly, \(\lambda_h^n = \sum_{E \in \mathcal{E}_h} \lambda_E^n w_E\) where \(X_K\) and \(X_E\) denote the characteristic functions of the element \(K\) and the face \(E\). They are defined on \(\Omega\) and \(\mathcal{E}_h\), respectively, and equal to one on \(K\) and \(E\), respectively, and zero elsewhere. By \(\{w_E\}\) we denote the set of basis functions of \(V_h\). We recall that the normal components \(v_h \cdot v\) of the fluxes on the faces are the degrees of freedom of functions \(v_h \in V_h\); cf. [16]. We further introduce

\[
B_{K,EE} = \int_K w_{K,E} \cdot w_{K,E} \, dx,
\]

\[
b_K = \sum_{E \in \mathcal{E}K} B_{K,EE}^{-1} z_{K,E} = \int_K \nabla z \cdot w_{K,E} \, dx,
\]

where \(w_{K,E}\) is the restriction of \(w_E\) to \(K\). Since the row sum of the matrix \(B_{K,EE}^{-1}\) does not depend on the row, which follows from the next but one formula, the term \(b_K\) is written without the additional index \(E\). With the abbreviation

\[
B = \sum_E |E|^4 \left( |E|^2 - \sum_{E \neq E} |\tilde{E}|^2 \right),
\]

one computes for the two-dimensional case that

\[
B_{K,EE}^{-1} = 16|K| \left( \delta_{EE} \sum_{E \neq E} |\tilde{E}|^2 (|E|^2 - |E'|^2)
\]

\[
+ \delta_{EE}^2 \sum_{E \neq E} (\delta_{EE} + \delta_{EE} + 0.5)|\tilde{E}|^2 + |E|^2 |E'|^2
\]

\[
- \sum_{E \neq E} |\tilde{E}^h| |E|^2 \right) B^{-1}, \quad z_{K,E} = \frac{1}{3} (z_E - z_0),
\]

\[
b_K = 48|K| \left( \sum_E |E|^2 \right)^{-1} \left( 1 - 6B^{-1} \cdot \prod_E |E|^2 \right),
\]

where \(z_{E,E} = 1 - \delta_{EE}\), \(z_0\) is the midpoint of the triangle side \(E\) and \(z_0\) is the vector opposite to \(E\), that is, \(z_0 \not\in \mathcal{E}_h\). Clearly, \(B_{K,EE}^{-1}\) is the element \(EE'\) of the inverse matrix and not the reciprocal of \(B_{K,EE}\). Further, \(|K|\) is the area of the triangle \(K\) and \(|E|\) the length of the side \(E\). The summation over \(E\) has to be understood as for all \(E \subset \partial K\), and \(\tilde{E} : \tilde{E} \neq E\) as for all \(\tilde{E} \subset \partial K\) with \(\tilde{E} \not\in E\), \(\tilde{E} \subset \partial K\), etc.

Choosing the basis functions of \(W_h, V_h\) and \(M_h\) as test functions in (8), then the hybrid mixed finite element approximation (8) of (1)–(3) can be rewritten as the algebraic system

\[
\Theta(\psi_h^n) + \tau_n \sum_{E \in \mathcal{E}h} q_E^n w_E = \Theta(\psi_h^{n-1}),
\]

\[
\sum_{E \in \mathcal{E}h} B_{E,EE} q_{E,E} = K(\psi_h^n)(\psi_h^n - \lambda_h^n - z_{K,E})
\]

for all \(K \in \Pi_h\) and \(E \subset \partial K\). Further, we have

\[
\sum_{K \in \mathcal{H}_h} q_{K,E} = 0
\]

for all \(E \in \mathcal{E}_h\). We simplify (9) and (10) in two steps. Firstly, the second identity in (9) implies

\[
q_{K,E} = K(\psi_h^n) \sum_{E \in \mathcal{E}_h} B_{E,EE}^{-1} (\psi_h^n - \lambda_E^n - z_{K,E}).
\]
We substitute (11) into the first equation of (9) and (10). From the representation of \( z_{K,E} \) given above we obtain \( \sum_{E \in \Omega} z_{K,E} = 0 \). Therefore, no gravitational term arises in the resulting discrete continuity equation that thus can be rewritten as

\[
\sum_{E \in \Omega} \mathbf{z}_K^e = F(\mathbf{\psi}_K^n)
\]

for all \( K \in \mathcal{K}_h \), where \( F(\mathbf{\psi}_K^n) \) is defined by

\[
F(\mathbf{\psi}_K^n) = 3 \mathbf{\psi}_K^n + |K| \frac{\Theta_k(\mathbf{\psi}_K^n) - \Theta_k(\mathbf{\psi}_K^{n-1})}{\varepsilon_k b_k K(\mathbf{\psi}_K^n)}.
\]

Hence we have obtained a system of equations which consists of one equation per element and per face for the unknowns \( \mathbf{\psi}_K^n \) and \( \mathbf{\lambda}_K^n \). Eq. (12) implicitly defines the pressure head \( \mathbf{\psi}_K^n \). Assuming that the inverse function \( F^{-1} \) exists, (12) implies that \( \mathbf{\psi}_K^n = F^{-1}(\sum_{E \in \Omega} \mathbf{z}_K^e) \). The existence of \( F^{-1} \) is not obvious and may impose restrictions on the temporal and spatial step sizes of the discretization. For an analysis of the invertability of \( F \) we refer to [7,38]. Secondly, substituting this representation of \( \mathbf{\psi}_K^n \) in terms of the Lagrange multipliers into the flux conservation equation resulting from the first simplification step yields

\[
\sum_{K,E \in \Omega} K \left( F^{-1} \left( \sum_{E \in \Omega} \mathbf{\lambda}_K^n \right) \right) \sum_{E \in \Omega} B^{-1}_{KE} \left( F^{-1} \left( \sum_{E \in \Omega} \mathbf{z}_K^e \right) - \mathbf{\lambda}_K^n - z_{K,E} \right) = 0
\]

for all \( E \in \partial_h \setminus \partial_h^D \). Thus we get the system

\[
G_E(\mathbf{\tilde{z}}_h^e) = 0
\]

for all \( E \in \partial_h \setminus \partial_h^D \) where \( G_E \) is defined by the left-hand side of (14). Here \( \mathbf{\lambda}_h^e = (\mathbf{\lambda}_E^n, \mathbf{\lambda}_D^n)^T \) with \( \mathbf{\lambda}_E^n = (\mathbf{\lambda}_E^n)_{E \in \partial_h \setminus \partial_h^D} \) and \( \mathbf{\lambda}_D^n = (\mathbf{\lambda}_E^n)_{E \in \partial_h^D} \) is the vector of the Lagrange multipliers. Since we require \( \mathbf{\lambda}_h^e \in M_{h,e} \), we have \( \mathbf{\lambda}_h^e = \mathbf{E}^{-1} \int_E g E d \sigma \) for \( E \in \partial_h^D \).

In every time step, the global nonlinear system (15) has to be solved for the Lagrange multipliers \( \{\mathbf{\lambda}_E^n\}_{E \in \partial_h \setminus \partial_h^D} \). For this a damped version of Newton’s method, Armijo’s rule (cf. [29]), is used. In the Newton steps the resulting linear system is solved by a multigrid method. Based on an equivalence of nonconforming and mixed finite element methods, the multigrid method is built from intergrid transfer operators derived for the lowest-order Crouzeix–Raviart element; cf. [10,21]. Namely, for linear elliptic problems

\[
-\nabla \cdot (A \nabla u) = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial \Omega,
\]

where \( A(x) \) is a symmetric, uniformly positive definite, bounded tensor and \( f \in L^2(\Omega) \) it has been shown (cf., e.g., [4,20]) that the mixed finite element method is equivalent to an augmented nonconforming Galerkin method. The modified nonconforming method yields a positive definite problem. However, various bubble functions have been used to prove the equivalence between the two methods. In the particular case of the lowest-order Raviart–Thomas element it has been established in [21] that the linear system which arises from the mixed finite element discretization of (16) is algebraically condensed to a positive definite system for the Lagrange multipliers is identical to the system arising from the standard nonconforming finite element method if a minor modification of the usual mixed method with the projection of the coefficients \( A^{-1} \) (component-by-component) and of the nonconforming method with the projection of the right-hand side \( f \) into the space \( W_h \) of piecewise constant functions is introduced. Hence, the equivalence between the mixed and nonconforming methods holds without adding any bubble functions. This induces us to apply the intergrid transfer operators constructed for the lowest-order Crouzeix–Raviart element (cf. [10] for details) to our algebraically condensed system of the hydrid mixed finite element approximation. No bubble functions are used in the implementation of the multigrid algorithm designed for the linear problems of the Newton iteration. We use the \( \mathcal{V} \)-cycle multigrid method. For problem (16) its convergence and approximation property is shown in [21]. While we have not found any proof for the convergence of the \( \mathcal{V} \)-cycle multigrid method, the results of our numerical experiments favorably indicate also its convergence. The difference between standard multigrid convergence results for nonconforming finite elements by, e.g., Braess and Verfürth (cf. [10]) and for the modified usual mixed finite element method is the projection of \( A^{-1} \) and \( f \) into the space \( W_h \). For the \( \mathcal{W} \)-cycle multigrid method the standard techniques can be carried over by a careful handling of the modified coefficients whereas they can not be applied to \( \mathcal{V} \)-cycle multigrid methods; cf. [21]. Finally, the results of [13] indicate the multigrid convergence even for nonsmooth solutions as they arise for the Richards equation; cf. Section 2.

In our multigrid method the coarse grid matrices are defined by a customary approximation of the Galerkin product. Its non-vanishing entries which link degrees of freedom on edges of different elements are added to the diagonal element of the respective row. The linear problem on the base level of the grid hierarchy is solved by LU decomposition. On the fine grid levels we use standard pre- and postsmoothers like Gauss–Seidel or ILU (cf. [29]). In our performed computations of subsurface flow the Gauss–Seidel smoother has shown to be, usually, the more robust alternative.

To apply Newton’s method to the system (15), we need the Jacobian \( A(\mathbf{\tilde{z}}_h^e) = (\partial G)/{(\partial \mathbf{\tilde{z}}_h^e)} \) which we compute analytically. We assume that
\[ \frac{\partial F}{\partial \psi_k^n} = 3 + |K|(\tau_n b_k K(\psi_k^n)^{-1}) - K'(\psi_k^n)(\Theta(\psi_k^n) - \Theta(\psi_k^{n-1})) \]

remains strictly positive. By choosing the time step size \( \tau_n \) sufficiently small we can ensure that the term \(-K'(\psi_k^n)(\Theta(\psi_k^n) - \Theta(\psi_k^{n-1})\)

in (17), which might potentially be negative, is sufficiently small and, thus, that \( \frac{\partial F}{\partial \psi_k^n} \) remains positive. Now, recalling (12), we compute that

\[ \frac{\partial \psi_k^n}{\partial \lambda_E^n} = \left( \frac{\partial}{\partial \psi_k^n} F(\psi_k^n) \right)^{-1} \]

where the term on the right-hand side is evaluated in \( \psi_k^n = F^{-1}(\sum_{E \subseteq K} \lambda_E^n) \). Together, (18) and (12) yield for the components \( A_{EE} \) of the Jacobian matrix \( A^t \) the identity

\[ A_{EE} = \sum_{K \in \pi_h} K(\psi_k^n) \left( -B_{K,EE}^{-1} + b_k + \frac{K'(\psi_k^n)}{K(\psi_k^n)} \right) \cdot \left( \frac{|K|}{\tau_n b_k} \right) \cdot \Theta(\psi_k^n) \left( \frac{K'(\psi_k^n)}{K(\psi_k^n)} \right) \sum_{E \subseteq K} (\psi_k^n - \lambda_E^n) \left( \frac{1}{\tau_n b_k} \right) \]

where the first summation has to be understood as for all \( K \in \pi_h \) with \( E \subseteq \partial K \) and \( E' \subseteq \partial K \).

In the \( i \)th Newton step where the iterate \( \lambda^{n(i)} \) is computed we thus solve the linear system \( A^0 c^{i(i)} = r^{i(i)} \) where \( A^0 \) is defined by \( A^0 = A(\lambda^{n(i-1)}) \), \( c^{i} \) the unknown correction and \( \rho^{i} = G(\lambda^{n(i-1)}) \) denotes the residual of the nonlinear system of equations (15). To compute \( r^{i} \) that is, to evaluate (15) for \( \lambda^{n(i-1)} \) we first have to determine the pressure \( P_{K}(\lambda^{n(i-1)}) = F^{-1}(\sum_{E \subseteq K} \lambda_E^{n(i-1)}) \) for all \( K \in \pi_h \) by solving element-wise the local problems (12). Again, this is done by Newton’s method applied to (12). Finally, the normal components \( d_{k,k'}^{n(i)} \) of the fluxes are calculated element-wise by (11).

5. Numerical convergence tests

In this section we shall analyze numerically the convergence rates of the proposed mixed hybrid finite element approximation of problem (1)-(3). For simplicity, this is done for the one-dimensional case \( \Omega \subseteq \mathbb{R} \) only. By an obvious appropriate interpretation of the boundary integrals, that is, by evaluating the integrands in the boundary points of the domain or element, respectively, the scheme can easily be rewritten for one space dimension. Since we are primarily interested in simulating two- and three-dimensional subsurface flows, this is not explicitly done here. The numerical results will figure out (cf. also [38]) that the expected theoretical convergence rates of the linear elliptic case (cf. [16]) can even be recovered for our nonlinear degenerate problem.

In the first computational experiment (cf. [27]) we consider a relatively simple formulation of the Richards equation which however is nonlinear and elliptic-parabolic degenerate. We use the parametrization \( \theta(\psi) = 2/(\pi/2 - \arctan(\psi)^2) \) and \( K(\psi) = 2/(1 + \psi^2) \) for \( \psi < 0 \) as well as \( \theta(\psi) = \pi^2/2 \) and \( K(\psi) = 2 \) for \( \psi \geq 0 \). Further, we suppose that \( \tau = 0 \). Thus, there is no gravitational force. Then Eq. (1) admits a travelling wave solution \( \phi(s) \), with \( s = x - \tau \), that is given by \( \phi(s) = -s/2 \) for \( s \leq 0 \) and \( \phi(s) = -\tan(\frac{\pi}{2} s) \) for \( s > 0 \). In our numerical calculations we use the data \( J \times L = (0.2 \times (0, 10)) \), \( \psi_0(x) = \phi(x) \) in \( \Omega \) as well as \( g_D(t, 0) = \phi(-t) \) and \( g_D(t, 10) = \phi(10 - t) \) for \( t > 0 \). At the initial time \( t = 0 \) the interface between the saturated and unsaturated region coincides with the left boundary and the domain \( \Omega \) is unsaturated. At the final time \( T = 2 \) the subdomain \( (0, 2) \) is saturated. We choose discretization parameters \( \tau \in [0.001, 0.1] \) and \( h \in [0.001, 1.0] \) and compute the \( L^2 \)-error between the exact and the numerical solution (8) at \( T = 2 \). Precisely, for the discretization parameters and within their respective intervals we use the three values \( 10^i, 2 \times 10^i \) and \( 5 \times 10^i \) for every order of magnitude \( i \), with \( i = -3, -2, -1, 0 \). The resulting errors \( ||\psi - \psi_h||_{L^2(\Omega)} \) and \( ||q - q_h||_{L^2(\Omega)} \), respectively, at \( T = 2 \) are visualized in Fig. 1. The x-axis gives the spatial step sizes \( h(a,c) \) and the temporal step sizes \( \tau(b,d) \), respectively. The convergence order of the discretization error is indicated by the slope of the respective triangle. We clearly observe first order convergence in space and time for the pressure variable \( \psi \) and also first order convergence rate for the temporal discretization of the flux variable \( q \). This is in complete agreement with theoretical results proven for linear elliptic problems; cf., e.g., [16]. Further we observe second order convergence for the spatial discretization of the flux \( q \) although a first order rate is only predicted for the lowest order Raviart–Thomas element by error analyses; cf., e.g., [16]. However, the second order convergence is due to the fact that we are in one space dimension. Here, \( RT_0 \) equals \( P_1(K) \) whereas in \( d > 1 \) dimensions \( RT_0 \) is a strict subspace of \( P_1(K)^d \). Further, if \( d = 1 \), the lowest order Raviart–Thomas and Brezzi–Douglas–Marini (BDM) element (cf. [16]) coincide and the lowest order BDM element is known to yield in fact second order convergence of the flux variable. Hence, the flux approximation is also consistent with theoretical results for linear elliptic problems. By an interpolation of the interelement Lagrange multipliers in the lowest order Crouzeix–Raviart space (cf. Section 7), a second order accurate approximation of the primal variable \( \psi \) is obtained; cf. [16]. This superconvergence result is also
confirmed by our calculations. We omitted the plots since they are similar to those in Fig. 1. Moreover, since the flux and piecewise constant pressure approximation are computed in terms of the Lagrange multipliers in a postprocessing procedure and since their convergence rates are in complete agreement with linear elliptic theory, it seems to be obvious that the convergence of the Lagrange multipliers also has to be of optimal order.

Our second example is more complex. We simulate the infiltration of a vertical soil column. Gravitation is included by putting $z = x$. We let $J \times \Omega = (0, 2000) \times (0, 1)$, $\psi_0(x) = -1 - x$ as well as $g_D(t, 0) = -1$ for $t > 0$ and $g_D(t, 1) = -2 + 0.022t$ for $0 < t < 100$ and $g_D(t, 1) = 0.2$ for $t > 100$. Here, length is measured in meter and time in seconds. For the parametrization of $\Theta(\psi)$ and $K(\psi)$ we use the model of van Genuchten and Mualem; cf. [26,34]. To dispel any question of parameter choice, we explicitly give the functional forms for $\Theta(\psi)$ and $K(\psi)$ and the parameters which we used in our computations. This shall allow one to compare directly own results with those of our computations. Precisely, for $\psi < 0$ they read as

$$
\Theta(\psi) = \Theta_i + (\Theta_s - \Theta_i) \theta, \quad \theta = (1 + (-\psi)^n)^{-m}
$$

$$
k_{rw}(\Theta(\psi)) = \sqrt{\eta(1 - (1 - \theta^{1/m})^2)},
$$

$$
K(\psi) = K_i k_{rw}(\Theta(\psi)), \quad m = 1 - 1/n.
$$

Here, $\theta$ denotes the relative saturation, $\Theta_i$ is the residual water content and $\Theta_s$ is the saturated water content. We consider soil characterized by the parameters $\Theta_i = 0.084$, $\Theta_s = 0.362$, $\alpha = 2.0$, $n = 2.0$ and $K_i = 1.25 \times 10^{-5}$ [m/s]. An analytical solution is not available anymore.

Therefore, we first determine a reference solution on a fine grid with $\tau = 2.0 \times 10^{-3}$ and $h = 1.0 \times 10^{-4}$ that is visualized in Fig. 2 for $t = 0$, 100 and 2000. Then we compute the difference of the solutions calculated on a sequence of coarser meshes to the reference one. Similarly to the previous example, this is done for the discretization parameters $10^i$, $2 \times 10^i$, $5 \times 10^i$, $i = 0, -1, \ldots$, in the intervals $\tau \in [0.1, 0.5]$ and $h \in [2 \times 10^{-5}, 0.1]$. The resulting errors at time $T = 2000$ are shown in Fig. 3.

Within the range of convergence, that is, for sufficiently small values of $h$ and $\tau$, respectively, we nicely observe the same convergence rates as in the first example. In Fig. 3c and d we omitted the range of very small step sizes, since for these values the accuracy of the reference solution is not high enough. Hence, we conclude that the convergence rates established in the literature for linear elliptic problems may even be obtained for nonlinear degenerate problems.

![Fig. 1. Pressure (a, b) error $\|\psi - \psi_h\|_{L^2(\Omega)}$ and flux (c, d) error $\|q - q_h\|_{L^2(\Omega)}$ over spatial (a, c) and temporal (b, d) step size for travelling wave solution at time $T = 2$.](image1)

![Fig. 2. Calculated profiles of pressure (a) and flux (b) at time $T = 0$, 100 and 2000 for the second of the infiltration problems.](image2)

![Fig. 3. Pressure (a, b) error $\|\psi - \psi_h\|_{L^2(\Omega)}$ and flux (c, d) error $\|q - q_h\|_{L^2(\Omega)}$ over spatial (a, c) and temporal (b, d) step size for numerical reference solution at time $T = 2000$.](image3)
6. Two-dimensional test problems

For our two-dimensional numerical tests of the proposed mixed hybrid finite element approximation we use the setting of a water table recharge problem which is illustrated in Fig. 4. The domain $\Omega$ is a box of 3 m height in gravitational direction and 2 m width. At time $t = 0$ we assume $\psi_0(x_1, x_2) = -x_2$ where the $x_i$, $i = 1, 2$, denote the components of $x$ and $x_2$ is the vertical direction against the gravitational force such that $\nabla z = (0, 1)^T$ in (1). On the boundary segment $\Gamma_1$ we prescribe $g_D(t, x) = -2\psi_0 + 2(\psi_0 + \psi_1)t/t_D$ for $t \leq t_D$ and $g_D(t, x) = 2\psi_1$ for $t > t_D$. On $\Gamma_2$ we set $g_D(t, x) = -\psi_0 x_2$. The data are compatible in the sense that $\psi_0(x) = g_D(0, x)$ on $\Gamma_1$ and $\Gamma_2$ which is physically reasonable and not really limiting. In this way we avoid inherent numerical instabilities due to incompatibilities between the initial and boundary conditions. Alternatively, if the solution lacks regularity as $t$ goes to zero, one may overcome the numerical difficulties resulting from this singular behavior at $t = 0$ by choosing (much) smaller (time) step sizes for the first time steps. At the rest of the boundary we prescribe the zero flux boundary condition $g_N(t, x) = 0$. This amounts to a symmetry line at the left side of the box and an impermeable layer for the ground water at the bottom. Thus, the flux $q$ becomes discontinuous at the right boundary of the segment $\Gamma_1$ and the upper boundary of the segment $\Gamma_2$. On $\Gamma_2$, the boundary condition holds the ground water table constant in depth 2 m.

In our first test the box is filled with clay. Time is measured in days. We choose $\psi_0 = 0$, $\psi_1 = 0.1$ and $t_D = 1$ (day) in the initial and boundary condition. The initial state is a hydrostatic equilibrium with vanishing flux $q = 0$. For the parametrization of $\Theta(\psi)$ and $K(\psi)$ we use the model of van Genuchten and Mualem; cf. Section 5 and [34, 26]. We consider Beit Netofa clay characterized by the $\Theta_s = 0$, $\Theta_e = 0.446$, $n = 0.152$, $r = 8.2 \times 10^{-4}$ [m/d]; cf. [26]. $K'(\psi)$ is not Lipschitz-continuous in $\psi = 0$ and is unbounded in the neighborhood of the saturated limit. Following a suggestion in [25], we replace $K(\psi)$ by a cubic spline interpolant in a neighborhood of the saturated limit for $0.99 \leq \theta \leq 1$.

Fig. 5 shows the results of our simulation based on the mixed hybrid finite element approach. In our computations we use the coarse mesh shown in Fig. 4 which is four times uniformly refined. This amounts to $74 \times 4^4 = 18,944$ elements. The multigrid solver then works on the hierarchy of the four grids thus obtained.

We use a constant time step size of $\tau_n = 0.05$ (day) for simplicity since we do not focus in this paper on the adaptivity for the temporal discretization. Our experiments with smaller time step sizes did not lead to any significant changes. In Fig. 5 we observe that a sharp interface between the unsaturated and saturated region occurs when water infiltrates the soil. The sharpness of the interface depends not only on the depth of the unsaturated region, given here by the initial condition, but also strongly on the soil properties, that is, the constants of the parametrization for $\Theta(\psi)$ and $K(\psi)$. Here, the constant $n$ in the van Genuchten and Mualem model (cf. Section 5) is chosen rather small which leads to the sharp transition zone and makes the problem hard to solve.

In our second experiment (cf. [30]) the box is filled with sand. Now, time is measured in seconds. We choose $\psi_0 = 3$, $\psi_1 = 0.6$ and $t_D = 50$ (s). Hence, the flux is not vanishing any more at $t = 0$. We use a time step size of $\tau_n = 0.5$ (s) for $t \leq 500$ (s), $\tau_n = 1.0$ for $500 < t \leq 1500$ and $\tau_n = 2.0$ for $t > 1500$. Here, the time step size is only increased to save compute time and demonstrate the stability of the suggested approximation scheme. Choosing smaller time step sizes did not lead to any significant changes in the computed results. For the parametrization of $\Theta(\psi)$ and $K(\psi)$ we use a model presented in [35]. For $\psi < 0$ it reads as

\[ g(\psi) = \begin{cases} 
\frac{\psi}{\psi_0} & \text{for } 0 \leq \psi < \psi_0 \\
\frac{-\psi_0}{\psi_0} & \text{for } \psi \geq \psi_0 
\end{cases} \]
\[ H_\text{h} = H_r + \left( H_s - H_r \right) \left( 1 + \left( -z \psi \right)^n \right)^{-1}, \]

\[ K(\psi) = K_0 \left( 1 + \left( -\beta \psi \right)^m \right)^{-1}. \]

We choose \( H_r = 0.075, \) \( H_s = 0.3, \) \( z = 2.71, \) \( n = 3.96, \)
\( \beta = 2.0, \) \( m = 4.74 \) and \( K_0 = 10^{-4} \text{ [m/s]} \).

Fig. 6 shows the results of our simulation. Again, we obtain a stable approximation of problem (1)–(3). Thus, the mixed hybrid finite element methodology leads to a powerful approach to handle the nonlinear degenerate problems of unsaturated–saturated flow.

7. Derivation of error indicators and adaptive mesh refinement algorithm

In particular our first test problem in Section 6 has shown that steep saturation fronts occur as water infiltrates dry soil. In order to resolve these fronts with a reasonable number of degrees of freedom and high accuracy, a local mesh refinement of the triangulations is inevitable for variably saturated subsurface flow problems. In this section shall present an error control mechanism for the mixed hybrid finite element approximation of problem (1)–(3). Our approach leads to error indicators in contrast to sharp error estimators verified by a rigorous mathematical analysis such that somewhat heuristic arguments may be allowed in the following. However, all performed calculations have led to convincing results and the error indicators are rather easy and fast to evaluate.

The strategies for error control and mesh refinement used in the finite element context are mostly based on a posteriori error estimates in global norms which involve local residuals of the computed solution. The resulting mesh refinement process then aims at equilibrating these local error indicators. For mixed finite element discretizations of linear elliptic problems Wohlmuth and Hoppe [42,43] have recently derived and analyzed four different kinds of a posteriori error estimators: a residual based estimator, a hierarchical one, error estimators relying on the solution of local subproblems and on superconvergence results. By similar techniques Carstensen [17] has also established a residual based estimator. The estimators generalize the standard concepts for a posteriori error estimators of the standard primal formulation to the mixed setting. For an excellent comparison of different kinds of error estimators in the conforming setting we refer to the work of Verfürth [41].

The investigation of the mixed approach is more complicated and requires some additional tools. Our approach relies on the residual and the superconvergence based a posteriori estimator of Wohlmuth and Hoppe which we apply to our nonlinear degenerate problem (1)–(3). They can be easily calculated by means of the available finite element approximations. In contrast to the hierarchical estimator, no additional subproblems have to be solved which seems attractive for numerical calculations. Controlling the accuracy in space by a posteriori error estimators constructed for stationary problems is a standard technique for dealing with parabolic ones; cf. [9,31,32]. Moreover, our performed computations of subsurface flow and infiltration problems have borne out that the spatial discretization error usually dominates the temporal one. Our computed results have shown not to be strikingly sensitive to changes in the time step sizes; cf. Section 6. In the special case of the superconvergence based error estimator, the fundamental error estimates on which the estimator relies can be re proven for the spatial discretization of a quite general class of parabolic problems; cf. [7]. Together, this may be considered as a motivation or, even, justification of our heuristic approach.

Another possibility to control the error is to discretize simultaneously in space and time employing a discontinuous Galerkin method and to apply coupled space–time estimators; cf. [24]. Such a posteriori estimators exist and have been rigorously analyzed for standard discretizations but not for mixed finite element methods of Raviart–Thomas type and degenerate problems. Moreover, since an additional dual problem has to be solved, the efficient implementation of these estimators is of fundamental importance and a demanding task. For the future we are planning to incorporate global residual based error control mechanisms relying on such concepts. However, currently we follow the first more heuristic approach which leads to simple error indicators. The resulting numerical approximations are stable and robust as our examples in Section 8 confirm.
First, we give now an error indicator for the primal variable \( \psi \) based on a superconvergence result. For this we recall that the multiplier technique that we have applied in Section 3 has two significant advantages. The first one is related to the specific structure of the resulting system of equations and the impact on the efficiency of the solution process as shown in Section 3 and 4. The second advantage is some sort of a super-efficiency of the solution process as shown in Section 3.

To explain the fundamental superconvergence result we consider, for simplicity, the linear elliptic problem (16). We introduce the space of lowest order Crouzeix–Raviart finite elements,

(23) gives rise to upper and a lower bounds for the discretization error of the primal variable \( u \) in the \( L^2 \) norm,

\[
\beta_1 \| u - \hat{u}_h \| \leq \| u - \psi_h \| \leq \beta_2 \| u - \psi_h \|
\]

(24)

with \( \beta_1 = (1 + 1)^{-1} \) and \( \beta_2 = (1 - 1)^{-1} \). Then the error estimator \( \eta_{S,u} \) is given as follows:

\[
\eta_{S,u} = \sum_{k \in \mathcal{N}_h} \| \hat{u}_h - u_0 \|_{L^2(K)}.
\]

Clearly, condition (23) is used to ensure that the error \( \| u - \hat{u}_h \| \) can be bounded below and above in terms of \( \| u - \psi_0 \| \) implying the reliability and sufficiency of the estimator \( \eta_{S,u} \). An equivalence between \( \| u - \hat{u}_h \| \) and a weighted sum of the squared jumps of \( u_0 \) across the edges \( E \in \mathcal{L}_0 \) can be established; cf. [43]. This is of importance if the original mixed system instead of its hybrid form is solved such that \( \hat{u}_h \) is not available without solving additional local problems.

We return to the approximation of the subsurface flow problems (1)–(3). Eq. (1) degenerates to an elliptic equation in the fully saturated regime and remains parabolic in the unsaturated one. Therefore, considering the degenerate case as a perturbation of the saturated one and proceeding in almost exactly the same way as before, we make the following saturation assumption:

For \( n = 1, \ldots, N \) there exists some constant \( c_n \) with \( 0 \leq c_n < 1 \) such that

\[
\| \psi(t_n) - \hat{\psi}_h^n \| \leq c_n \| \psi(t_n) - \psi_0^n \|.
\]

Here \( \psi(t_n) \) denotes the solution of (1)–(3) at time \( t_n \) and \( \hat{\psi}_h^n \in CR_{h,n} \) is the nonconforming extension of \( \hat{\lambda} \) defined analogously to (19) by \( \int_E (\psi_h - \hat{\psi}_h^n) \, d\sigma = 0 \) for all \( E \in \mathcal{L}_0 \).

The fundamental convergence results (20) and (22) that justify the assumption (23) and (25), respectively, may be violated for a combination of Dirichlet and Neumann boundary conditions or, in particular, our nonlinear degenerate problem where the solution lacks enough regularity. Nevertheless, we may realistically expect that they hold at least in some sense locally such that the saturation assumption (25) remains reasonable. This might be sufficient for our local error estimation and grid refinement strategies and lead to a good working error indicator. We shall see. Further, we note that the estimates (20) and (22) can be reproven for the semidiscretization in space of a quite general class of parabolic problems with sufficiently regular solution; cf. [7]. If the fully discretized problem is considered, of course, an additional term of the order \( \mathcal{O}(h) \) arises in the error estimates where \( h \) denotes the time step size. If \( k \) is of the order \( \mathcal{O}(h^r) \), then the superconvergence result (22) even holds for the fully discretized mixed finite element approximation of such parabolic problems. Of course, such severe restriction of the time step sizes would not be efficient for computations, and it is also not necessary as our performed calculations confirm; cf. Section 8. This may be due to the minor importance of the temporal
discretization error already mentioned above. Our error indicator (cf. (26)) is solely based on the saturation assumption (25). No further restriction is used. Finally, we note that the saturation assumption is formulated in terms of the pressure head \( \psi \) and not the hydraulic head \( \phi + z \) since \( \psi \) represents the primal variable of our formulation and we aim to control its approximation error by an indicator. Alternatively, we could formulate a saturation assumption for the hydraulic head \( \phi + z \) by adding projections of \( z \) onto the spaces \( CR_h \) and \( W_h \) to \( \psi_h^n \) and \( \psi_h^s \), respectively. This is not done here.

Using the triangle inequality, assumption (25) directly gives rise to the following upper and lower bounds for the \( L^2 \)-discretization error of \( \psi \),

\[
c_{n1} \left\| \psi_h^n - \psi_h^s \right\| \leq \left\| \psi(t_n) - \psi_h^n \right\| \leq c_{n2} \left\| \psi_h^n - \psi_h^s \right\|
\]

with \( c_{n1} = (1 + c_n)^{-1} \) and \( c_{n2} = (1 - c_n)^{-1} \). Then the superconvergence based error indicator \( \eta_{S,\psi} \) for the pressure head is given as (\( \| \cdot \| = \| \cdot \|_{L^2(K)} \))

\[
\eta_{S,\psi} = \sum_{K \in \mathcal{I}_h} \eta_{S,\psi,K}^2, \quad \eta_{S,\psi,K} = \left\| \psi_h^n - \psi_h^s \right\|.
\]  

Employing the trapezoidal quadrature rule, the local error indicator \( \eta_{S,\psi,K} \) can be rewritten as

\[
\eta_{S,\psi,K}^2 = \frac{1}{3} \left| K \right| \sum_{E \in \partial K} (\tilde{\psi}_h^E - \psi_h^s)^2.
\]  

The terms on the right-hand side of this identity are available without any additional computations. The vector \( \tilde{\psi}_h^E = (\tilde{\psi}_h^E)_{E \in \partial K} \) is the vector of the unknowns of the global nonlinear system of equations which is solved in each time step. The piecewise constant approximations \( \psi_h^s \) are computed locally in the Newton iterations when the residual of the nonlinear system of equations is evaluated; cf. Section 4. Hence, \( \eta_{S,\psi,K} \) is rather easy and fast to compute. We recall that the basic estimates (20), (22) hold in two and three dimensions such that (26) may be applied in both cases.

So far, we have provided a superconvergence based error indicator for the primal variable \( \psi \) of our flow problems (1)-(3). For the mixed formulation (7) it is natural to ask whether the error in the flux variable \( q \) can be estimated and controlled similarly. Then, by superposition we get an error indicator for the total error. This seems possible by using a result of Brandts [11]. To explain it, we restrict ourselves to the two-dimensional case \( \Omega \subset \mathbb{R}^2 \). An extension to three space dimensions seems possible but has not been completely investigated and tested yet. For simplicity, let us first consider the linear elliptic problem (16) again. We further suppose that the triangulation \( \mathcal{I}_h \) is uniform which means that two adjacent triangles of \( \mathcal{I}_h \) form a parallelogram; cf. [11]. Of course, this will be violated in an adaptive grid refinement process. We will return to this later. We introduce the operator \( J_h : V_h \rightarrow CR_h \) which is locally given by its value at the midpoint \( m_E \) of the triangulation

\[
J_h p_h(m_E) = 0.5 \cdot (p_h|_K + p_h|_{K'}) (m_E),
\]

with \( E = K \cap K' \), if \( E \in \partial_1 \) is an interior edge. Since \( V_h \subset H(\text{div}; \Omega) \) is satisfied, the normal components to edges of functions \( v_h \in V_h \) are continuous across those edges of triangles. Hence, the operator \( J_h \) is actually only postprocessing the tangential components here. If we are dealing with a boundary edge, that is, one which has only a triangle \( K \) on one side of that edge, then there exists, due to our assumption, at least one \( K' \in \mathcal{I}_h \) such that \( K \cup K' \) is a parallelogram. The straight line through the midpoint \( m_E \) of the boundary edge and the center \( m_C \) of the parallelogram intersects the boundary of \( K \cup K' \) in another point \( m_p \). We will assume that \( J_h p_h \) is already defined at \( m_C \) and \( m_p \) of at least one of the parallelograms \( K \cup K' \) associate to \( K \). Then we choose such a parallelogram and define the value of \( J_h p_h \) in \( m_E \) by linear extrapolation

\[
J_h p_h(m_E) = 2J_h p_h(m_C) - J_h p_h(m_p).
\]  

Let now \( u \in W^2_2(\Omega), p = -A \nabla u \) denote the solution of the equations (16). Then, for a uniform and regular triangulation there holds (cf. [11])

\[
\| p - J_h p_h \| \leq c h^{2/3} \| p \|_{W^2_3(\Omega)}
\]  

for the Dirichlet problem as well as

\[
\| p - J_h p_h \| \leq c h^2 \| p \|_{W^2_3(\Omega)}
\]  

for the homogeneous Neumann problem where \( p_h \) is the mixed (hybrid) finite element approximation of \( p \). Recalling (21), we see that \( J_h p_h \) provides a higher order approximation of \( p \) than \( p_h \).

We now proceed in exactly the same way as for the pressure. Motivated by the a priori estimates (21), (29) and (30), we make the following saturation assumption:

There exists some constant \( 0 \leq \beta < 1 \) such that

\[
\| p - J_h p_h \| \leq \beta \| p - p_h \|.
\]  

Again, (31) gives rise to upper and lower bounds for the \( L^2 \)-discretization error of \( p \),

\[
\beta_1 \| J_h p_h - p_h \| \leq \| p - p_h \| \leq \beta_2 \| J_h p_h - p_h \|
\]

with \( \beta_1 = (1 + \beta)^{-1} \) and \( \beta_2 = (1 - \beta)^{-1} \). The error estimator \( \eta_{S,p} \) is then given as

\[
\eta_{S,p}^2 = \sum_{K \in \mathcal{I}_h} \eta_{S,p,K}^2, \quad \eta_{S,p,K} = \| J_h p_h - p_h \|_{L^2(K)}.
\]

It is easy to see that \( \eta_{S,p} \) as well as \( \eta_{S,p} \) is an asymptotically exact error estimator, that is, the quotient of the error estimator and the error itself converges to 1 when \( h \) tends to zero.

We return to problems (1)-(3). In an adaptive grid refinement process the above-made uniformity assumption about the triangulation which is fundamental for
the convergence rate estimates (29) and (30) is usually violated. The rationale for using nevertheless the following approach based on (29) and (30) comes in the numerical results; cf. Section 8. First, the extrapolation (28) for boundary edges has to be redefined. The straight line through the midpoint $m_E$ of the boundary edge $E$ and the midpoint $m_{E'}$ of another edge $E'$ of the triangle $K$ intersects the element $K'$ adjacent to $E'$ in some point $p_{E'}$ on $E' \neq E$ that is not necessarily the midpoint of $E$. The operator $\tilde{J}_h$ is then defined analogously to $J_h$, now with linear extrapolation from $m_{E'}$ and $p_{E'}$. Motivated by (21), (29) and (30), we make the saturation assumption:

For $n = 1, \ldots, N$ there exists some constant $c_n$ with $0 \leq c_n < 1$ such that

$$
\|q(t_n) - \tilde{J}_h q_h^k\| \leq c_n \|q(t_n) - q_h^k\|.  
$$

(32)

Here $q(t_n)$ denotes the solution of (2)–(5) at time $t_n$. Our superconvergence based error indicator for the flux $q$ is then given by ($\|\cdot\|_1 = \|\cdot\|_{L^2(K)}$)

$$
\eta_{S,q,E}^2 = \sum_{K \in \mathcal{TH}_h} \eta_{S,q,E,K}^2, \quad \eta_{S,q,E,K}^2 = \|q_h^k - \tilde{J}_h q_h^k\|.  
$$

(33)

Again, (32) ensures the existence of lower and upper bounds for $\|q(t_n) - q_h^k\|$ in terms of $\|q_h^k - \tilde{J}_h q_h^k\|$. Employing the trapezoidal quadrature rule, the term $\eta_{S,q,E,K}$ can be rewritten as

$$
\eta_{S,q,E,K}^2 = \frac{1}{3} \sum_{K \in \mathcal{TH}_h} |K| \left( \int_{\partial K} (q_{h} - \tilde{J}_h q_{h})^2 \right)^{1/2}.  
$$

In the parabolic case a superconvergence result for the flux $q$, similarly to (29) and (30), can be proven for the semidiscretization in space with respect to the norm of $L^2(J; L^2(\Omega))$; cf. [7]. This would require a time-integrated saturation assumption and lead to a posteriori error estimator for the totalized error ($\sum_{j=0}^{n} \alpha_j \|q(t_j) - q_h^k\|^2$) with some weights $\alpha_j$ depending, in particular, on the time step sizes $\tau_j$. Nevertheless, we use the non-integrated version (32) of the saturation assumption, primarily, since we aim to apply the a posteriori error estimator of the stationary case also to parabolic and degenerate problems and, secondly, since computations have shown that (33) leads to more robust results than its corresponding totalized counterpart.

Finally, we give a residual based indicator for the total error $\|\psi(t_n) - \psi_h^k\| + \|q(t_n) - q_h^k\|_{H(\Omega; \text{div})}$ for simplicity, we first consider the linear elliptic problem (16) again. We further suppose that $A$ is a piecewise constant diagonal matrix. The basic idea behind the construction of the residual based error estimator is to use the Helmholtz decomposition of the flux space $H(\Omega; \text{div})$,

$$
H(\Omega; \text{div}) = H^0(\Omega; \text{div}) \oplus H^1(\Omega; \text{div}),  
$$

where $H^0(\Omega; \text{div}) = \{q \in H(\Omega; \text{div}) | \nabla \cdot q = 0\}$ and $H^1(\Omega; \text{div}) = \{q \in H(\Omega; \text{div}) | (A^{-1}q, g^h) = 0 \forall g^h \in H^0(\text{div}; \Omega)\}$; cf. [17,43]. According to this splitting, the flux error can uniquely be written as $p_e = p_e^0 + p_e^1$ where $p_e^0 \in H^0(\Omega; \text{div}; \Omega)$ and $p_e^1 \in H^1(\Omega; \text{div}; \Omega)$. The mixed variational problem satisfied by the error $(u_v, p_v) = (u - u_h, b - p_h)$ can then be decomposed into two independent subproblems which are treated separately. The first subproblem is associated with the solenoidal subspace and gives rise to the problem (cf. [43])

$$
\langle A^{-1}p_e^0, v \rangle = r(v) \quad \text{for all } v \in H^0(\text{div}; \Omega),  
$$

(34)

where the residual $r$ is given by $r(v) = -(A^{-1}p_v, v) + \langle \nabla \cdot v, u_h \rangle$. From (34) it follows (cf. [43]) that

$$
\sum_{E \in \mathcal{TH}_h} w_E \|\pi_{k_E} (A^{-1}p_v \cdot \zeta)\|^2_{L^2(E)} \text{ yields sharp upper and lower bounds for the solenoidal part } p_e^0 \text{ of the flux error.}
$$

Here, $h_E$ denotes the length of the edge $E$ and $\zeta$ is the unit tangential vector on $\partial K$ obtained by rotating the outer normal $\nu$ on $\partial K$ by $\pi/2$ counterclockwise. Let $x^h_0$ and $x^h_1$, $0 < x^h_0 < x^h_1$, be the local bounds of the coefficient matrix $A$ defined by $x^h_1 |x| \leq x^h_0 |x|$, $x \in \mathbb{R}^3$, for almost all $x \in K$. Then, the weighting factors $x_E$ are defined by $x_E := (x^h_1(x^h_0 - x^h_1)/2 + x^h_0)$ and $w_E = 1/2$ if $E \in \partial K \cap \partial K_2$ is an interior edge, and by $x_E := (x^h_1(x^h_0 - x^h_1)/2 + x^h_1)$ and $w_E = 1$ if $E \subset \partial K \cap \partial \Omega$. The jump $[\cdot]$ on the interior edge $E = \partial K_1 \cap \partial K_2$ is defined by $[A^{-1}p_v \cdot \zeta] = A^{-1}p_v \cdot \zeta|_{K_1} - A^{-1}p_v \cdot \zeta|_{K_2}$, and on the boundary edge $E \in \partial K \cap \partial \Omega$ as $[A^{-1}p_v \cdot \zeta] = A^{-1}p_v \cdot \zeta|_{K}$. To obtain a sharp estimate for $p_v$, in a second step the term $p_v^1$ is considered. Recalling $\nabla \cdot p_v = \nabla \cdot p_v^1$, the mixed approximation of (16) also yields

$$
\langle \nabla \cdot p_v^1, w \rangle = \langle f - P_0 f, w \rangle \quad \text{for all } w \in L^2(\Omega),  
$$

(35)

where $P_0 f$ denotes the $L^2$-projection of $f$ onto $W_h$. Eq. (35) readily provides a lower and upper $L^2$-bound for $\|\nabla \cdot p_v^1\|$ and, moreover, using a norm equivalence on $H^1(\Omega; \text{div})$, also for $p_v^1$ in terms of $\|f - P_0 f\|$; cf. [43] for details. The error $u_v$ in the primal variable is then bounded above and below by making use of the preceding estimates and standard duality techniques. Precisely, the residual based error estimator proven in [43] for a piecewise constant diagonal matrix $A$ reads as

$$
\eta_{R,u,p}^2 = \sum_{K \in \mathcal{TH}_h} \eta_{R,u,p,K}^2,  
$$

$$
\eta_{R,u,p,K}^2 = \|f - P_0 f\|^2_{L^2(K)} + h_K^2 \|A^{-1}p_v \cdot \zeta\|^2_{L^2(K)}  
$$

$$
+ \sum_{E \in \mathcal{TH}_h} w_E h_E \|A^{-1}p_v \cdot \zeta\|^2_{L^2(E)},  
$$

where $h_K$ the diameter of $K$. Again, an error estimator is obtained which can be easily calculated by means of the available finite element approximations of the primal variable and the flux. No additional subproblems have to be solved. In the special case of the Poisson equation with homogeneous Dirichlet boundary conditions the sum $\eta_{S,u} + \eta_{R,u}$ of the superconvergence based estimator for the primal variable and the flux is locally equivalent with the residual based error estimator; cf. [43]. Hence, we may expect similar meshes for the either indicators.
For our subsurface flow problems (1)–(3) the corresponding indicator reads as \( \| \cdot \| = \| \cdot \|_{L^2(K)} \)

\[
\eta_{R,\psi',\phi'} = \sum_{K \in H_0} \eta_{R,\psi',\phi',K}, \\
\eta_{R,\psi',\phi',K}^2 = |z - P^w_0|^2 + h^2_K |K(\psi')^{-1} q^n_k|^2 \\
+ \sum_{E \in \partial K} w_E z_E h_E \left[ |K(\psi')^{-1} q^n_k|^2 \right]_{L^2(E)}
\]

with \( w_E \) and \( z_E \) being defined analogously to the elliptic case. The formulation of the error indicator again relies on our approach to apply systematically the error estimator of the linear elliptic regime also to parabolic and degenerate problems.

Finally, it remains to describe our adaptive mesh refinement algorithm; cf. also [6]. As input this algorithm receives a hierarchy \( P = \{ P^m \}_{m=0}^\infty \) of simplicial triangulations of \( \Omega \) on which the linear problem of the Newton iteration is solved (cf. Section 4) and where the leaf elements (those without sons) have been tagged with a refinement rule or a coarsening tag. Here, we use the well known refinement process due to Bank et al. [5]. The refinement rule is such that a triangle \( K \in P^K_h \), 0 \( \leq j \leq m \), either remains unrefined, or is subdivided into four congruent subtriangles, or is bisected into two subtriangles. Following the refinement in [5], each triangle \( K \in P^K_h \) is geometrically similar either to an element of \( P^K_h \) or to a bisected triangle of \( P^K_h \). If all sons of an element are tagged for coarsening, they are deleted from the data structure. Of course only leaf elements can be removed, since coarsening should be an inverse operation to refinement. A high-level version of the global refinement algorithm reads as:

\[
\text{RefineMultiGrid}(P^m, m) = \\
\text{for} \quad l = m, m - 1, \ldots, 1 \\
\quad \text{MakeConsistent}(P^m_h) \\
\quad \text{RestrictTags}(P^l_h, P^{l-1}_{h-1}) \\
\quad \text{for} \quad l = 0, 1, \ldots, m \\
\quad \text{MakeConsistent}(P^l_h) \\
\quad \text{DetermineCopies}(P^l_h) \\
\quad \text{RefineGrid}(P^l_h) \\}
\]

The overall structure of the algorithm RefineMultiGrid resembles a multigrid \( \gamma \)-cycle. The first for-loop proceeds from the top level \( m \) to level 1. No manipulation of the data structure is done in this first loop, only the refinement tags are manipulated. The function MakeConsistent computes a consistent grid for level \( l + 1 \) by tagging elements of level \( l \) with the refinement rule. Function RestrictTags computes the influence of level-\( l \)-tags on level-(\( l - 1 \))-tags. In the second loop the data structure is actually modified proceeding from coarse to fine levels. When the second loop is entered, the grid on level \( l \) has already been modified and level \( l + 1 \) is constructed from tags stored on level \( l \). Again Make-

Consistent is called to compute consistent tags. Then DetermineCopies computes the algebraic classes which in turn determine the copy elements required on level \( l + 1 \). The function RefineGrid actually modifies the data structure. Appropriate objects are created/deleted on level \( l + 1 \). After completion the function Refine-Multigrid has constructed a new multigrid hierarchy. Its top level is either \( m - 1, m \) or \( m + 1 \). Intergrid transfer operators for systems with element- and edgewise degrees of freedom are defined and analyzed in [12]. In [12], the prolongation of the edge values is independent of the element values. Therefore, we instead use the prolongation given in [10] for the lowest-order Crouzeix–Raviart element; cf. Section 4. Restriction is the adjoint mapping. The intergrid transfer operator for the elementwise degrees of freedom is defined by averaging; cf. [12].

For local tagging of the elements \( K \) of a grid \( P^K_h \) of the hierarchy \( P \), the elementwise contributions \( \eta^K \) of the respective error indicator \( \eta_{S,\psi',\phi'} \) or \( \eta_{R,\psi',\phi'} \), respectively, are computed. An element \( K \in P^K_h \) is tagged for coarsening if \( \eta^K |K|^{-1/s} < \sigma \cdot e \), where \( e \) is a prescribed accuracy and \( \sigma \) is a tolerance that is typically chosen in \( [10^{-1}, 1] \). The factor \( \sigma \) inhibits the coarsening of the elements and, thereby, prevents spurious oscillations in the grid generation process. The element \( K \) is tagged for refinement if \( \eta^K |K|^{-1} > e \). If \( \sigma \cdot e \leq \eta^K |K|^{-1} \leq e \), \( K \) remains unmodified.

The adaptive mesh refinement algorithm is applied only once before a time step is performed except for the initial time where an iteration between setting of the initial value and grid adaptation is done. This seems to be a practicable and an efficient approach. The result is in fact a good working error indicator as the simulations in Section 8 confirm. Computations have shown that iterating in each time step strongly increases the compute time, but does not lead to any significant changes in the adaptively generated grids. Further, it should not be forgotten, that our adaptive techniques lead to error indicators in contrast to mathematically rigorous estimators. Of course, the error indicators may also be applied in an iterative way which means that every time step is recomputed on a modified grid until the (local) error indicators satisfy the prescribed tolerances.

8. Adaptive simulations

For the numerical test of our error indicators and mesh refinement algorithm we recompute the first of the water table recharge problems of Section 6. At the initial time, the coarse grid (level zero) of the multigrid algorithm is generated by subdividing all triangles of the mesh shown in Fig. 4 into four congruent subtriangles. In either experiments (cf. Fig. 7), the iteration at \( t = 0 \) between setting of the initial value and grid adaptation
leads to an additional global refinement step, that is, subdivision of all triangles of the coarse mesh into four subtriangles. In the subsequent time steps the multigrid solver then works on an adaptively generated hierarchy of grids, and the number of levels may vary from time step to time step. In our computations coarsening is only done from level one on upwards. Thus, the grid on level zero remains uncoarsened. In our computations of typical subsurface flow we made the experience that the performance properties of the nonlinear and linear solver are improved if the grid on the lowest level is not chosen too coarse. This seems reasonable since we have to resolve sharp fronts. If the grid on the lowest level is too coarse, then these fronts are not approximated with sufficient accuracy on the lowest level which seems to increase the complexity of the solution process. However, we found no indication that this observation is really limiting the problem size. In our calculations the algorithm remained stable even for quite coarse lowest level grids and steep fronts.

In our first simulation the superconvergence based error indicator (27) is applied. The required tolerance $\varepsilon$ is chosen as $\varepsilon = 1.5e^{-3}$. Fig. 7 shows the results of our simulation. We observe the expected sharp resolution of the interface between the saturated and unsaturated zone. The local strong refinement at the right boundary of $\Gamma_1$ and the upper boundary of $\Gamma_2$ (cf. Fig. 4) is supposed to be due to the transition of the boundary condition from Dirichlet type to Neumann type in those points with a discontinuity of the flux and a singular behavior of the solution there. Choosing a smaller tolerance $\varepsilon$ leads to a further global refinement step at $t = 0$, and this additional global refinement is essentially preserved at succeeding times. Outside a neighborhood of the interface between the two zones the adaptive computation (cf. Fig. 7) was done on a much coarser mesh than the calculation in Section 6, with two refinements of the coarse grid now instead of four global refinements in Section 6. This saves compute time. In the computed pressure profiles we do not observe any significant differences although the mesh is now much coarser in the predominant part of the box. But, we do see a change in the approximation if the tolerance for the adaptive mesh refinement is weakened. A slowdown of the movement and smearing of the saturation front resulting from an insufficient resolution of the transition region can be observed. This indicates that we have a good working approach.

Our next simulation is devoted to a study of the residual based error indicator $\eta_K \psi, q$. Thus, we now aim to “control” the total error $\|\psi(t_n) - \psi^h_\ast\| + \|q(t_n) - q^h_\ast\|_{H(\text{div})}$. The required tolerance $\varepsilon$ is chosen as $\varepsilon = 4.0e^{-4}$. Fig. 7 shows the results of our simulation. Again, the interface between the zones is resolved. But now, the saturated flow region behind the interface is stronger refined than in the previous case where only an error indicator for the pressure was considered. This seems reasonable since in the saturated region the variation in the pressure is low (see isolines in Fig. 5) and, therefore, the pressure based error indicator does not demand a mesh refinement there. The strong refinement of the saturated region behind a moving front by an indicator for the total error can also be observed in the results of Starke [39,40] which are based on an error estimator for the total error of a least-squares mixed finite element approximation of the Richards equation. Hence, if an accurate computation also of the saturated region is required, then the residual based error

![Fig. 7. Superconvergence based error indicator for pressure (top) and residual based error indicator for pressure and flux: Top level of adaptively refined triangulations for $T = 1, 2, 5, 10, 20, 40$ (days).](image-url)
indicator seems to be superior to the superconvergence based indicator for the pressure. Otherwise, for applications in which only the position of the saturation front is of importance, the superconvergence based error indicator seems to be sufficient and more efficient. Similarly to the previous case, we observe a local strong refinement at the right boundary of \( \Gamma_1 \) and the upper boundary of \( \Gamma_2 \) due to the change of the type of the boundary conditions there.

If the adaptive grid generation is based on the sum of the superconvergence based error indicators \( \eta_{S,\psi} \) and \( \eta_{S,q} \) for pressure head \( \psi \) and flux \( q \), we obtain grids quite similar to those of the previous case (cf. Fig. 7) in which the flow region behind the interface is again stronger refined than in the first case. However, since \( \eta_{S,q} \) is typically much smaller than \( \eta_{S,\psi} \), one has to weight the two terms by considering \( c_1 \eta_{S,\psi} + c_2 \eta_{S,q} \) with some fixed constants \( c_1 \) and \( c_2 \). The equivalence of the grids does not seem to be surprising due to the above-mentioned known local equivalence of the error estimators for the Poisson equation.

Finally, we shall show that the proposed adaptive algorithm is in fact superior to a computation on a uniform mesh. This is done by comparing the resulting discretization errors. For simplicity, we consider a one-dimensional problem. We recompute the second of the examples of Section 5. It is done for the temporal step size \( \tau = 0.1 \) only. For spatial discretization parameters \( h \in [2 \times 10^{-4}, 0.1] \) we calculate the \( L^2 \)-error of the pressure by comparing the approximate solutions obtained on these meshes to the reference solution calculated on a very fine grid; cf. Section 5. This is done for the time \( t = 100 \) and 2000. The adaptive computations are performed with tolerance \( \sigma = 1/6 \) and for accuracy parameters \( \varepsilon \in [10^{-7}, 10^{-2}] \). Precisely, within the respective interval of \( h \) and \( \varepsilon \) we choose the values \( 10^i \), \( 2 \times 10^i \) and \( 5 \times 10^i \) for every order of magnitude \( i = -1, -2, \ldots \). In the adaptive simulations we use the superconvergence based error indicator \( \eta_{S,\psi} \) for the pressure. The approximation errors over the number of elements are visualized in Fig. 8. Similar plots are obtained for the residual based indicator.

We nicely observe that the adaptive calculations lead to smaller discretization errors over the whole range and, thus, have an advantage over the uniform computations. At \( t = 100 \) this difference is more significant than at \( t = 2000 \) which is due to the fact that the pressure profile is much steeper at \( t = 100 \). It is resolved more accurately by the adaptive distribution of the finite elements. In the left plot the curves approach a constant number for \( h \to 0 \) which is due to the dominating temporal discretization error in this range.

9. Conclusions

We think that these numerical results show the effectiveness of the adaptive mixed hybrid finite element approach for the nonlinear degenerate problems arising in variably saturated subsurface flow. In particular, the results of our computational tests demonstrate two favorable properties: (i) the use of the proposed heuristic based error indicators which are easy and fast to evaluate without solving additional (sub-)problems leads to a good working adaptive mesh refinement algorithm, and (ii) the Newton and multigrid method are robust schemes to solve the resulting nonlinear system of equations. The mixed hybrid finite element methodology thus leads to a powerful approach to handle the nonlinear degenerate problems in saturated–unsaturated subsurface flow.

Acknowledgements

The authors thank the referees for their suggestions for improving the presentation of the paper.

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