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A robust linearization scheme for finite volume based discretizations for simulation of two-phase flow in porous media

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Abstract

In this work we consider a mathematical model for two-phase flow in porous media. The fluids are assumed immiscible and incompressible and the solid matrix non-deformable. The mathematical model for the two-phase flow is written in terms of the global pressure and a complementary pressure (obtained by using the Kirchhoff transformation) as primary unknowns. For the spatial discretization, finite volumes have been used (more precisely the multi-point flux approximation method) and in time the backward Euler method has been employed. We present here a new linearization scheme for the nonlinear system arising after the temporal and spatial discretization. We show that the scheme is linearly convergent. Numerical experiments are presented and sustain the theoretical results.

Keywords: two-phase flow, linearization schemes, finite volume, MPFA, convergence analysis.

1. Introduction

Among the numerous applications of two-phase flow in porous media we mention water and soil pollution, CO₂ storage, enhanced oil recovery and nuclear waste management. These applications relate to problems of strong interest for the society and underline the high relevance of understanding of two-phase flow in porous media. A crucial role in understanding two-phase flow in porous media is played by numerical simulations, including mathematical modelling and numerical methods.

Mathematical models of two-phase flow in porous media consist of coupled, nonlinear and possibly degenerate partial differential equations. This makes the design and implementation of efficient numerical schemes for two-phase flow in porous media a challenging task. Locally conservative discretizations such as finite volume [1, 11, 12, 15, 22] and mixed finite element [6, 4] methods are popular spatial discretization as they alleviate many stability issues. Furthermore, as long time-scales are of frequent interest in applications, fully implicit temporal discretizations are, in general, preferred.

The spatial and temporal discretization thus leads to a large system of nonlinear equations for each time step. This system is usually solved by either Picard's method [17] or Newton's method [5, 17, 23, 24, 25]. The former is linearly convergent while the latter is quadratically convergent. The quadratic convergence of Newton's method comes at the price of only local convergence in solution space, however it remains a very powerful tool when applied to systems arising from

discretization of parabolic equations. This is because, in this case the starting iteration is chosen as the solution at the last time step and the initial error can be controlled. In this way, by adjusting the time step size one ensures that the starting iteration is in the convergence region of the method. In order to apply Newton's method to degenerate problems one needs a further regularization step [23, 24, 25], which may alter the quality of the solution. Moreover, the time-step restriction depends on the mesh diameter and on the size of the regularization step, which may be relatively restrictive in practice (see [24, 25] for *a priori* derived convergence conditions for the Newton method when applied to transport equations). Thus, we identify two main concerns of Newton's method: the need for regularization for degenerate problems, as well as the time-step constraint implicitly imposed by the convergence region.

In this work we propose and analyse a new linearization scheme for finite volume discretization schemes for two-phase flow. The proposed scheme is a monotone fixed point iteration [21, 26]. We can show that the scheme is linearly convergent and very robust (subject to a relatively mild restriction on the time step size but independent of grid size). Moreover, the scheme does not involve the calculation of derivatives, which is an advantage over both Picard and Newton methods. Our analysis and numerical experiments indicate that the new scheme is a valuable alternative to Picard or Newton method for solving two-phase flow in porous media.

The paper is structured as follows. In Section 2, we present the two-phase model considered here, describe the linearization scheme and show its convergence. The numerical results are given in Section 3, which show the applicability of the method. The paper ends with some concluding remarks in Section 4.

2. Mathematical model and discretization

In this work we consider a simplified mathematical model for two-phase flow in porous media. The fluids are assumed immiscible and incompressible and the solid matrix is assumed non-deformable. The formulation adopted here uses the global pressure and a complementary pressure (obtained by using the Kirchhoff transformation) as primary unknowns (see [8, 9]). For simplicity of exposition, we will furthermore assume spatially homogeneous relative permeability and capillary pressure functions, and an absence of gravity.

Throughout this paper we will use common notations from functional analysis. The domain $\Omega \subset \mathbb{R}^d$, d being the dimension of the space, is assumed to be open, bounded and with a Lipschitz continuous boundary. By C we mean a positive constant, not depending on the unknowns or the discretization parameters.

2.1. Governing equations

Mass (volume) balance:

$$\frac{\partial s(\theta)}{\partial t} + \nabla \cdot \vec{q}_w = f_1, \quad (1)$$

Fractional phase flux

$$\vec{q}_w = -k \nabla \theta + f_w(s) \vec{q}. \quad (2)$$

Conservation of total phase volumes

$$\nabla \cdot \vec{q} = f_2. \quad (3)$$

Darcy's law for total flow

$$\vec{q} = -\lambda(s) k \nabla p \quad (4)$$

The equations hold true in $\Omega \times [0, T]$, with T denoting the final time. It is understood that these equations are completed by constitutive laws for the various functions f , as well as an invertible

relationship between the saturation s and the complementary pressure θ . The system (1)-(4) to be solved includes two coupled nonlinear partial differential equations, one degenerate elliptic - parabolic and other elliptic for which, as previously remarked, the existence and uniqueness of a solution has been proved in [9]. Initial and boundary conditions complete the model.

2.2. Assumptions on the data

Throughout this paper we consider the following physically reasonable assumptions on the data and the solution of the continuous problem.

(A1) $s(\cdot)$ is monotone increasing and Lipschitz continuous.

(A2) The permeability $k > 0$ and the total mobility $\lambda(\cdot)$ is Lipschitz continuous and there exists $a_*, a^* \in \mathbb{R}$ such that for all $y \in \mathbb{R}$, it holds true

$$0 < a_* \leq \lambda(y) \leq a^* < \infty. \quad (5)$$

(A3) $f_1(\cdot)$, $f_2(\cdot)$ and $f_w(\cdot)$ are Lipschitz continuous and bounded functions.

2.3. Temporal discretization

Let $N \geq 1$ be an integer giving the time step $\Delta t = T/N$, and let $t_n = n\Delta t$, for $n = 1, \dots, N$ the discrete time points. A fully implicit temporal discretization of equations (1) leads to the nonlinear system of equations wherein the variables in equations (2)-(4) are evaluated at time t^n while equation (1) becomes

$$s^n + \Delta t(\nabla \cdot \vec{q}_w^n - f_1) = s^{n-1}. \quad (6)$$

2.4. Iterative approach

The standard approach to solving equations (2)-(6) is to apply Newton's method. As mentioned in the introduction, this has several drawbacks. First, the Jacobian matrix of the system needs to be assembled, and secondly, the convergence of the algorithm is not guaranteed when the initial guess is not "close enough", which implies a restriction on the time-step. We consider therefore the applicability of a linearization method. Let

$$L = \sup_{\theta} \frac{d}{d\theta} s(\theta). \quad (7)$$

In practice, any constant $L \geq \sup_{\Theta} \frac{d}{d\Theta} s(\Theta)$ will ensure the convergence of the scheme. Then iterate i is obtained by solving the following system of equations

$$L(\theta^{n,i} - \theta^{n,i-1}) + s^{n,i-1} + \Delta t(\nabla \cdot \vec{q}_w^{n,i} - f_1) = s^{n-1} \quad (8)$$

$$\vec{q}_w^{n,i} = -k\nabla\theta^{n,i} + f_w(s^{n,i-1})\vec{q}^{n,i} \quad (9)$$

$$\nabla \cdot \vec{q}^{n,i} = f_2 \quad (10)$$

$$\vec{q}^{n,i} = -\lambda(s^{n,i-1})k\nabla p^{n,i} \quad (11)$$

Note that this system is decoupled, in the sense that equations (10)-(11) and (8)-(9) can be solved sequentially. Thus, only one global (elliptic or parabolic) system needs to be solved at a time.

2.5. Spatial discretization

Equations (8)-(11) have previously been solved in the context of mixed finite element approximations to the spatial derivatives. Here, in contrast, we consider a finite volume setting. We introduce a finite volume duplex $\mathcal{D} = (\mathcal{T}, \mathcal{F})$, representing the mesh Tessellation and Faces:

- \mathcal{T} is a non-overlapping partition of the domain Ω . Furthermore, let m_K denote the d -dimensional measure of $K \in \mathcal{T}$.
- \mathcal{F} is a set of faces of the partitioning \mathcal{T} . Naturally, the faces must be compatible with the mesh, such that for all $K \in \mathcal{T}$ there exists a subset $\mathcal{F}_K \in \mathcal{F}$ such that $\partial K = \cup_{\sigma \in \mathcal{F}_K} \sigma$.

Additionally, we state the following useful subsets of the mesh duplex, which allows us to efficiently sum over neighboring cells or faces:

- For each cell $K \in \mathcal{T}$, we denote the faces that comprise its boundary by \mathcal{F}_K .
- For each face $\sigma \in \mathcal{F}$, we denote the neighboring cells \mathcal{T}_σ . Note that for all internal faces \mathcal{T}_σ will contain exactly two elements, while it contains a single element when $\sigma \subset \partial\Omega$.

This is sufficient to provide an abstract definition of a finite volume method for equations (8)-(11). With respect to equations (8)-(11), we identify p and θ as cell variables and $q = \vec{q} \cdot \vec{n}$ as a face variable, and denote the corresponding discrete spaces as $\mathcal{H}_\mathcal{T}$ and $\mathcal{H}_\mathcal{F}$. It follows that s is also a cell variable.

A finite volume method is characterized by the existence of a discrete operator $\tilde{\nabla} \cdot : \mathcal{H}_\mathcal{F} \rightarrow \mathcal{H}_\mathcal{T}$ defined for each $K \in \mathcal{T}$ such that

$$(\tilde{\nabla} \cdot \vec{q})_K = \frac{1}{m_K} \sum_{\sigma \in \mathcal{F}_K} \pm m_\sigma q_\sigma \quad \text{for all } q \in \mathcal{H}_\mathcal{F}. \quad (12)$$

The choice of sign in equation (12) is determined by the convention on normal vectors for faces.

Various finite volume methods differ in their definition and construction of discrete operators representing equation (4), which we denote by $F(p, s) : (\mathcal{H}_\mathcal{T} \times \mathcal{H}_\mathcal{T}) \rightarrow \mathcal{H}_\mathcal{F}$. It is typical to consider this mapping as a product $F = F_1(p)F_2(s; F_1(p))$ where then $F_1 : \mathcal{H}_\mathcal{T} \rightarrow \mathcal{H}_\mathcal{F}$ and $F_2 : (\mathcal{H}_\mathcal{T} \times \mathcal{H}_\mathcal{F}) \rightarrow \mathcal{H}_\mathcal{F}$. Classically, F_1 is a discrete representation of a Darcy flux, while F_2 is a (potentially smoothed) upstream value of the function $\lambda(s)$.

The fully discrete scheme can then be written as: find $(\theta^{n,i}, p^{n,i}, \vec{q}^{n,i}) \in \mathcal{H}_\mathcal{T} \times \mathcal{H}_\mathcal{T} \times \mathcal{H}_\mathcal{F}$ such that

$$L(\theta^{n,i} - \theta^{n,i-1}) + s^{n,i-1} + \Delta t(\tilde{\nabla} \cdot \vec{q}_w^{n,i} - f_1) = s^{n-1}, \quad (13)$$

$$\vec{q}_w^{n,i} = F_1(\theta^{n,i}) + f_w(F_2(s^{n,i-1}; F_1(\theta^{n,i})))\vec{q}^{n,i}, \quad (14)$$

$$\tilde{\nabla} \cdot \vec{q}^{n,i} = f_2, \quad (15)$$

$$\vec{q}^{n,i} = F_1(p^{n,i})F(s^{n,i-1}; F_1(p^{n,i-1})), \quad (16)$$

where it is still understood that $s^{n,i-1} = s(\theta^{n,i-1})$. Equations (13) and (13) are understood elementwise for each $K \in \mathcal{T}$, while equations (13) and (13) hold for each face $\sigma \in \mathcal{F}$. Furthermore, note that equations (15)-(16) are a linear elliptic system, which is still decoupled from (13)-(14), which is itself a linear system.

2.6. Convergence of the iterative method

We introduce now the errors at the iteration step i :

$$e_\theta^{n,i} = \Theta_h^{n,i} - \Theta_h^n, e_p^{n,i} = p_h^{n,i} - p_h^n, e_s^{n,i} = s_h^{n,i} - s_h^n = s(\Theta_h^{n,i}) - s(\Theta_h^n).$$

In order to show the convergence of the scheme (13) - (16) we will prove that

$$\|e_\theta^{n,i}\|, \|e_p^{n,i}\| \rightarrow 0 \text{ when } i \rightarrow \infty,$$

where $\|\cdot\|$ stays as the notation for the discrete L_2 norm, $\|f\|^2 := \sum_{K \in \mathcal{T}} m_K |f_K|^2$. It follows that

also $\|e_s^{n,i}\| \rightarrow 0$. In the same spirit, we define also a discrete L_2 scalar product by $\langle f, g \rangle := \sum_{K \in \mathcal{T}} m_K f_K g_K$.

Theorem 2.1. *Assuming (A1)-(A3) and that the time step Δt is sufficiently small, and that the finite volume method satisfies (21), the linearization scheme (13) - (16) is (at least) linearly convergent.*

Proof. we will give the main idea of the proof, pointing out only what is peculiar for the convergence of the new scheme and assuming that the standard estimates can be obtained for the considered finite volume method. By subtracting equations (13) - (16) from (6) and (2)-(4) one gets

$$L(e_\theta^{n,i} - e_\theta^{n,i-1}) + e_s^{n,i-1} + \Delta t G_1(\theta^{n,i}, \theta^n, p^{n,i}, p^n, s^{n,i-1}, s^n) = 0, \quad (17)$$

and

$$\tilde{\nabla} \cdot G_2(p^{n,i}, p^n, s^{n,i-1}, s^n) = 0, \quad (18)$$

with the expressions G_1 and G_2 depending on the considered finite volume scheme. By standard techniques one can assume that (18) implies

$$\|e_p^{n,i}\| + \|\bar{q}^{n,i} - \bar{q}^n\| \leq C_0 \|e_s^{n,i-1}\|, \quad (19)$$

with C_0 not depending on the discretization parameters. We multiply now (17) with $e_\theta^{n,i}$ (the multiplication is done element wise, and after weighing by the cell volume m_K then summed up) to obtain

$$L\langle e_\theta^{n,i} - e_\theta^{n,i-1}, e_\theta^{n,i} \rangle + \langle e_s^{n,i-1}, e_\theta^{n,i} \rangle + \Delta t \langle G_1(\theta^{n,i}, \theta^n, p^{n,i}, p^n, s^{n,i-1}, s^n), e_\theta^{n,i} \rangle = 0. \quad (20)$$

We need the following inequality for the finite volume method, which can be easily verified (see the following section):

$$\langle G_1(\theta^{n,i}, \theta^n, p^{n,i}, p^n, s^{n,i-1}, s^n), e_\theta^{n,i} \rangle \geq C_1 \|e_\theta^{n,i}\|^2 - C_2 \|e_s^{n,i-1}\|^2 - C_3 \|e_p^{n,i}\|^2 \quad (21)$$

where C_1 is not depending on Δt and C_2, C_3 are not depending both on Δt and mesh size. Putting together now (19) - (21), and some algebraic manipulations we obtain

$$\left(\frac{L}{2} + C_1 \Delta t\right) \|e_\theta^{n,i}\|^2 + \frac{L}{2} \|e_\theta^{n,i} - e_\theta^{n,i-1}\|^2 + \langle e_s^{n,i-1}, e_\theta^{n,i} \rangle \leq \frac{L}{2} \|e_\theta^{n,i-1}\|^2 + \Delta t (C_2 + C_3 C_0) \|e_s^{n,i-1}\|^2. \quad (22)$$

By using the monotonicity of s , its Lipschitz continuity and the Young inequality, i.e. $|ab| \leq \frac{\epsilon}{2} |a|^2 + \frac{1}{2\epsilon} |b|^2$ for all $\epsilon > 0$ we further get

$$\begin{aligned} \left(\frac{L}{2} + C_1 \Delta t\right) \|e_\theta^{n,i}\|^2 + \frac{L}{2} \|e_\theta^{n,i} - e_\theta^{n,i-1}\|^2 + \langle e_s^{n,i-1}, e_\theta^{n,i-1} \rangle &\leq \frac{L}{2} \|e_\theta^{n,i-1}\|^2 \\ &+ \Delta t (C_2 + C_3 C_0) \|e_s^{n,i-1}\|^2 + \langle e_s^{n,i-1}, e_\theta^{n,i-1} - e_\theta^{n,i} \rangle, \end{aligned} \quad (23)$$

which implies

$$\begin{aligned} \left(\frac{L}{2} + C_1\Delta t\right)\|e_\theta^{n,i}\|^2 + \frac{1}{L}\|e_s^{n,i-1}\|^2 &\leq \frac{L}{2}\|e_\theta^{n,i-1}\|^2 \\ &+ \Delta t(C_2 + C_3C_0)\|e_s^{n,i-1}\|^2 + \frac{1}{2L}\|e_s^{n,i-1}\|^2. \end{aligned} \quad (24)$$

From (24) we immediately obtain

$$\left(\frac{L}{2} + C_1\Delta t\right)\|e_\theta^{n,i}\|^2 + \left(\frac{1}{2L} - \Delta t(C_2 + C_3C_0)\right)\|e_s^{n,i-1}\|^2 \leq \frac{L}{2}\|e_\theta^{n,i-1}\|^2, \quad (25)$$

which proves the convergence of the scheme under the mild assumption

$$\frac{1}{2L} - \Delta t(C_2 + C_3C) \geq 0,$$

which is a restriction on the time step size. We say that the assumption is 'mild' because the time step size restriction does not depend on the grid size, so it is by far not that restrictive as would be a stability condition when using an explicit scheme. ■

2.7. An appropriate finite volume method

For concreteness, we will consider MPFA-type discretizations to obtain the linear operator F_1 (see [1] for an introduction). These are constructed such that the support of q_σ is local (in terms of connectivity of \mathcal{D}). Furthermore, the MPFA discretizations have been shown to be robust and convergent for a range of relevant parameters and grids [16, 3]. While any of the established MPFA methods are applicable, our particular interest is a new MPFA method, recently proposed in [18], which is the scalar counter-part of the finite volume method for elasticity given in [19]. Convergence of the method is established in [18]. It remains to verify that inequality (21) holds.

Indeed, the existence of a positive constant C_1 follows from monotonicity of the method, which in the setting of finite volume methods will in general be dependent on grid and anisotropy. Sufficient [20] and necessary [13] conditions have been identified for Cartesian grids, and necessary conditions on triangular grids have also investigated [14]. The existence of coefficients C_2 and C_3 is a simple consequence of continuity of the discretization and the constitutive functions.

3. Numerical results

Using the scheme as described above, we consider the 2D and 3D domains as given respectively by the unit square and unit cube with Dirichlet boundary conditions. Our main aim is to provide a numerical verification of the results of Theorem 2.1.

As constitutive functions, we are motivated by coarse-scale models for CO₂ storage to consider linear relative permeability functions [7]. Using a mobility ratio of $m \neq 1$, the fractional flow function f_w thus becomes a ratio of linear functions. Furthermore, we consider a capillary pressure function on the form

$$p^{cap}(s) = c(s + (\lambda_c/\lambda_b - 1)^{-1} \ln(s)).$$

Here λ_b and λ_c are the end-point mobilities of the two (linear) phase mobility functions. This choice of capillary pressure function ensures that the complimentary pressure function is also non-linear, yet still analytically tractable:

$$s(\theta) = 1 - \left(1 - \frac{2(\lambda_c - \lambda_b)\theta}{c\lambda_c\lambda_b}\right).$$

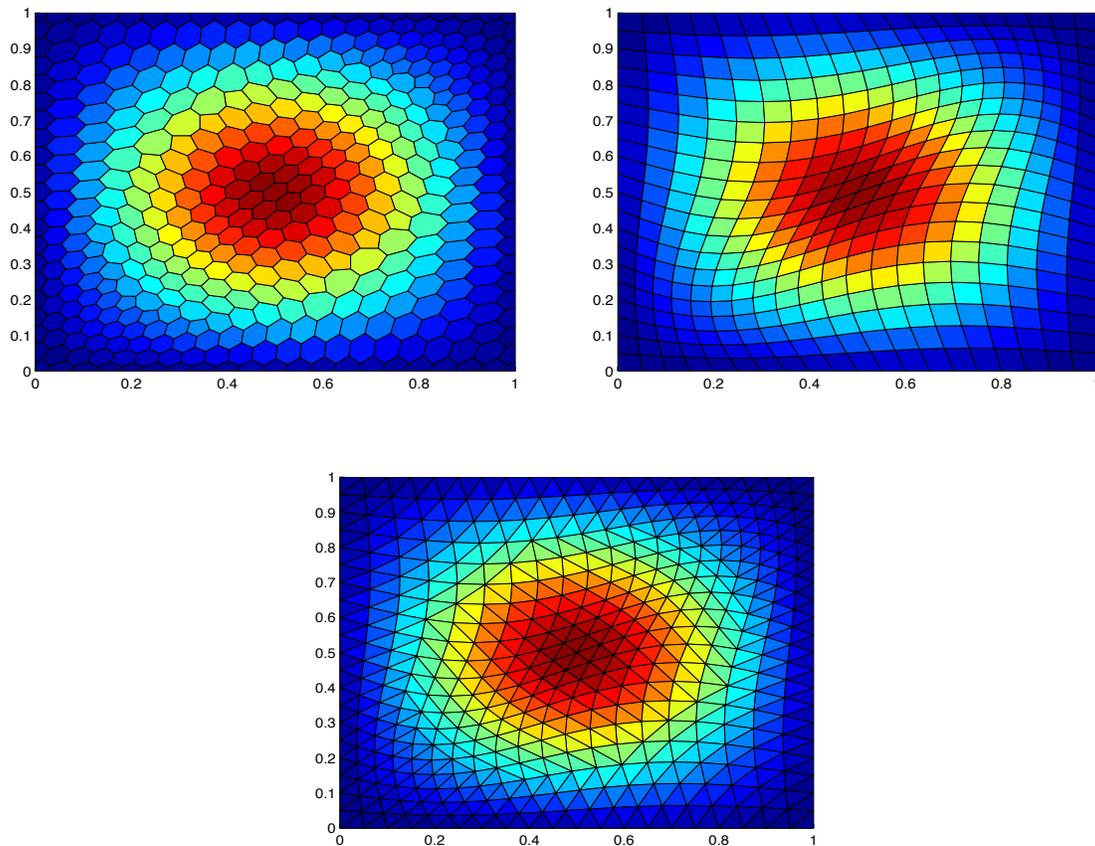


Figure 1: Example simulation results after 4 time steps on various grids. The use of an MPFA spatial discretizations yields very little grid orientation effects, while the combination of implicit time integration allows for long time steps.

By simple inspection we see that this leads to a Lipschitz constant of $L = c\lambda_c\lambda_b/(\lambda_c - \lambda_b)$. A typical simulation on various unstructured and structured grids is depicted in Figure 1. All simulations were conducted on a standard laptop using the Matlab implementation environment, and the total run-time for the test suite amounts to less than 10 minutes.

We consider grids varying from 400 to 10,000 cells in 2D and 3D. In all cases, we use a constant time-step of 0.1 (dimensionless units). For all simulations, we give a tolerance in residual error of 10^{-3} for the non-linear system. Throughout all numerical experiments we observe that the linear error reduction factor is stable between 3 and 8.5, independent of grid type, grid resolution, or dimensionality of the problem, as illustrated by the results shown in Figure 2. This implies that in no instance was more than a maximum of 7 iterations needed. Furthermore, the experiments support the assertion that no grid-dependent time-step restriction is introduced by the solution of the non-linear system. This verifies the robustness and generality of the iterative scheme, and the suitability of the finite volume discretization for complex geometries.

4. Conclusions

We presented in this work a new and robust linearization scheme for finite volume discretizations of two-phase flow in porous media. The scheme was shown to be linearly convergent if the time step is small enough. The restriction on the time step size is very mild compared to the stability condition for explicit temporal discretizations or with time step size restrictions for Newton's

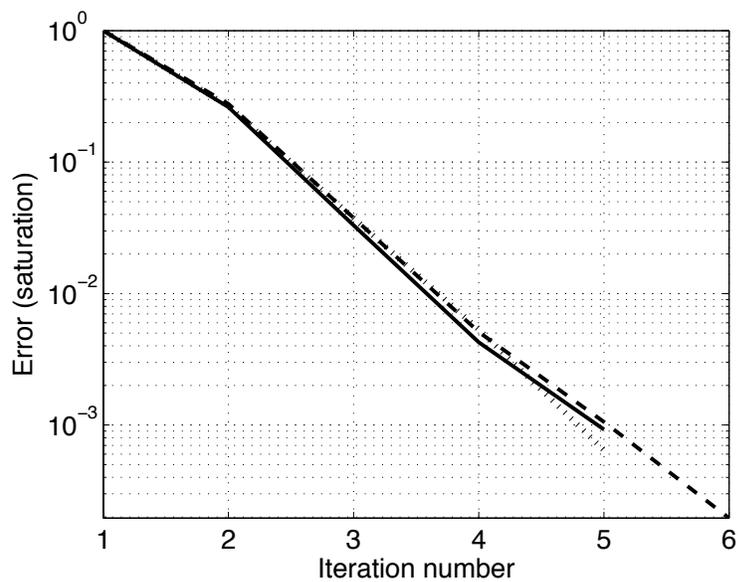


Figure 2: Convergence history of relative saturation error for the first time-step for various grids. Illustrated are 100x100 quadrilateral grid (solid line), triangular grid with 800 cells (dashed line), and a 3D unstructured grid with 3840 cells (dotted lines).

method. In the latter two cases the time step restriction depends on the mesh diameter, while for the new scheme the restriction is independent of it. Another advantage of the presented scheme is that it does not involve the calculations of derivatives. Numerical examples (both two and three dimensional) sustain the theoretical results. We especially remark that there is almost no difference in terms of number of iterations between the 2D and 3D computation, which is an argument for the efficiency of the scheme. The new numerical scheme is relatively simple to implement and is a valuable alternative to Picard or Newton methods.

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