A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows *

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October 18, 2011

Abstract

This paper develops a general abstract framework for a posteriori estimates of the dual norm of the residual for immiscible incompressible two-phase flows in porous media, enabling to control the overall error. Our estimators also allow to estimate separately the different error components, namely the spatial discretization error, the temporal discretization error, the linearization error, the iterative coupling error, and the algebraic solver error. We propose an adaptive algorithm wherein the different iterative procedures (iterative linearization, iterative coupling, iterative solution of linear systems) are stopped when the corresponding errors do not affect significantly the overall error, and wherein the spatial and temporal errors are equilibrated. Consequently, important computational savings may be achieved while guaranteeing a user-given precision. The developed framework covers fully implicit, implicit pressure–explicit saturation, or iterative coupling formulations; conforming spatial discretization schemes such as the vertex-centered finite volume method or the finite element method and nonconforming spatial discretization schemes such as the cell-centered finite volume method, the mixed finite element method, or the discontinuous Galerkin method; linearizations such as the Newton or the fixed-point one; and general linear solvers.

Key words: two-phase flow, a posteriori error estimate, general framework, discretization error, linearization error, iterative coupling error, algebraic solver error

1 Introduction

Let an open bounded polygonal (polyhedral) domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, and a time interval $(0, t_{\rm F})$, $t_{\rm F} > 0$, be given and set $Q := \Omega \times (0, t_{\rm F})$. We consider the immiscible incompressible two-phase flow in porous media in the form

$$\partial_t(\phi s_\alpha) - \nabla\cdot \left(\frac{k_{{\rm r},\alpha}(s_{\rm w})}{\mu_\alpha}\underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) = q_\alpha \qquad \text{in } Q,\ \alpha \in \{{\rm n}, {\rm w}\}, \tag{1.1a}$$

$$s_{\rm n} + s_{\rm w} = 1 \qquad \text{in } Q, \tag{1.1b}$$

$$p_{\rm n} - p_{\rm w} = p_{\rm c}(s_{\rm w}) \qquad \text{in } Q. \tag{1.1c}$$

*The first author was supported by the ERT project "Enhanced oil recovery and geological sequestration of CO_2: mesh adaptivity, a posteriori error control, and other advanced techniques" and by the GNR MoMaS. The second author was partially supported by the NSF-CDI under contract number DMS 0835745 and the Center for Frontiers of Subsurface Energy Security under Contract No. DE-SC0001114

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Here the unknowns are s_α, the *phase saturations*, and p_α, the *phase pressures*, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$. The subscripts n, w stand for nonwetting and wetting, respectively. Typically, the nonwetting phase is oil and the wetting one is water. For the sake of simplicity, we suppose that the porosity ϕ, as well as the phase viscosities μ_α and the phase densities ρ_α are all constant. The permeability tensor $\underline{\mathbf{K}}$ and the phase sources q_α, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, are only supposed to depend on the space coordinate $\mathbf{x}$ and on the time t. For the sake of simplicity, we suppose q_α piecewise constant in time on time mesh defined below. In (1.1a)–(1.1c), z stands for the vertical coordinate and g for the gravitation acceleration constant. The system (1.1a)–(1.1c) is nonlinear and coupled because of the presence of p_c, the capillary pressure, and of $k_{\mathrm{r},\alpha}$, the phase relative permeabilities, which are both given functions of the wetting phase saturation s_w. For example, in the Brooks–Corey [11] model,

$$k_{\mathrm{r,w}}(s_\mathrm{w}) = s_\mathrm{e}^4, \quad k_{\mathrm{r,n}}(s_\mathrm{w}) = (1 - s_\mathrm{e})^2(1 - s_\mathrm{e}^2)$$

and

$$p_\mathrm{c}(s_\mathrm{w}) = p_\mathrm{d} s_\mathrm{e}^{-\frac{1}{2}},$$

where

$$s_\mathrm{e} := \frac{s_\mathrm{w} - s_\mathrm{rw}}{1 - s_\mathrm{rw} - s_\mathrm{rn}}.$$

Here p_d is the entry pressure and s_rw and s_rn are respectively the wetting and nonwetting residual saturations. Note that (1.1a)–(1.1c) is degenerate as the phase relative permeabilities $k_{\mathrm{r},\alpha}$ can become zero.

Define the phase Darcy velocities $\mathbf{u}_\alpha$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, by

$$\mathbf{u}_\alpha := -\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha} \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha g \nabla z). \tag{1.2}$$

For the sake of simplicity only, we suppose homogeneous Neumann boundary conditions

$$\mathbf{u}_\alpha \cdot \mathbf{n}_\Omega = 0 \qquad \text{on } \partial\Omega \times (0, t_\mathrm{F}),\ \alpha \in \{\mathrm{n}, \mathrm{w}\}. \tag{1.3}$$

Conditions (1.3) can be replaced by more realistic ones. The initial condition is imposed through

$$s_\mathrm{w}(\cdot, 0) = s_\mathrm{w}^0 \qquad \text{in } \Omega \tag{1.4}$$

and we also fix

$$(p_\mathrm{w}(\cdot, t), 1) = 0 \qquad \forall t \in (0, t_\mathrm{F}), \tag{1.5a}$$

$$(q_\mathrm{n}(\cdot, t) + q_\mathrm{w}(\cdot, t), 1) = 0 \qquad \forall t \in (0, t_\mathrm{F}). \tag{1.5b}$$

Here and below, $(\cdot, \cdot)$ stands for the $L^2(\Omega)$ scalar product.

The problem (1.1a)–(1.5b) is of fundamental importance in petroleum engineering. Many results on this problem and on its numerical approximation have been derived in the past. The analysis of (1.1a)–(1.5b) including the existence, uniqueness, and well-posedness results has been in particular carried out in [40, 17, 5, 18, 19, 20, 13], see also [3, 45, 51]. For the use and analysis of mixed finite element methods for the numerical approximation of (1.1a)–(1.5b) we refer to, e.g., [23, 6, 58] and the references therein, for discontinuous Galerkin methods, to, e.g., [27, 28, 29] and the references therein, for cell-centered finite volume methods to, e.g., [34] and the references therein, and for vertex-centered finite volume methods to, e.g., [36] and the references therein. Multiscale and mortar techniques, efficient parallelization, and multinumerics and multiphysics formulations have been investigated in [48]. Linearization, linear solver techniques, and stopping criteria for multiphase flows are discussed in, e.g., [57, 42, 41].

The purpose of the present paper is to derive a posteriori estimates for numerical approximations of the problem (1.1a)–(1.5b). Our estimates give a guaranteed and fully and easily computable upper bound on the selected error measure, the dual norm of the residual augmented by the distance of the approximate global and complementary pressures to proper function spaces. Recall that such error measure leads to the energy error for linear problems (cf., e.g., [31]), and it is shown in [14] that this is an upper bound on the error between the exact and approximate saturations, global pressures, and complementary pressures for conforming discretizations. Our estimates also allow to distinguish, estimate separately, and compare different error components. The principal error component is the discretization error, due to the numerical scheme chosen, the local space mesh size, and the local time mesh size. This can be decomposed into *space discretization error* and *time discretization error*. The subsidiary error component is the error due to various iterative procedures involved in the calculation. This includes *linearization error*, *iterative coupling error*, or *linear solver error*. We next devise adaptive algorithms where all the iterative procedures on a given time level are stopped whenever the individual errors drop to the level at which they do not affect significantly the overall error. Simultaneously, the space and time discretization errors are adjusted so that they are of similar size.

The benefits of such a procedure are twofold. Firstly, the overall error is controlled and strategies for obtaining a user-given final precision at the end of the simulation can be devised. Secondly, it is likely to lead to important computational savings, as performing an excessive number of unnecessary linearization/iterative coupling/linear solver iterations and using too fine (with respect to the other components of the error) space or time meshes can be avoided. These concepts have been known for long time in the engineering practice but only recently, rigorous mathematical analysis has been started in model cases. In particular, linear solver error estimation and linear solver stopping criteria have been developed in, e.g., [9, 46, 7], nonlinear solver error estimation and nonlinear solver stopping criteria are treated in, e.g., [35, 15, 16], and spatial and temporal errors are estimated and balanced in, e.g., [49, 50, 52, 44]. Inexact Newton methods have been studied in, e.g., [24, 25]. Herein, we build upon the results of [37, 26, 31, 32] which give guaranteed and robust a posteriori estimates.

The present paper gives a posteriori error estimates in a very general setting without a specification of the underlying numerical treatment. Examples of the application of the present abstract framework to different discrete formulations, spatial and temporal discretizations, linearizations, and linear solvers are given in [21, 14]. In order to unify the presentation, we have chosen once and for all as the primary unknowns the pressure and saturation of the wetting phase. Adjustments to all other choices are easily possible.

2 Preliminaries

We specify here the notation and function spaces used, characterize the weak solution, give our assumptions on the approximate solutions, and define the error measure.

2.1 Function spaces and space and time meshes

We denote by $H^1(\Omega)$ the Sobolev space of those functions from $L^2(\Omega)$ which admit a weak gradient in $[L^2(\Omega)]^d$. The functions from $H^1(\Omega)$ are *continuous* in the trace sense, so that $H^1(\Omega)$ is a perfect mathematical space for representing continuous scalar physical quantities. A counterpart of $H^1(\Omega)$ for vector functions is the space $\mathbf{H}(\mathrm{div}, \Omega)$ of those functions from $[L^2(\Omega)]^d$ which admit a weak divergence in $L^2(\Omega)$. The functions from $\mathbf{H}(\mathrm{div}, \Omega)$ have a *continuous normal trace* (in appropriate sense), so that $\mathbf{H}(\mathrm{div}, \Omega)$ is a perfect mathematical space for representing mass-conservative vector physical quantities. We will also need below the space

$$X := L^2(0, t_{\rm F}; H^1(\Omega)); \tag{2.1}$$

for $\varphi \in X$, we set

$$\|\varphi\|_X := \left\{ \int_0^{t_{\rm F}} \|\nabla \varphi\|^2 {\rm d}t \right\}^{\frac{1}{2}}$$

and observe that X is the usual energy space for parabolic problems and that $\|\varphi\|_X$ is the associated energy norm.

We consider a strictly increasing sequence of discrete times $\{t^n\}_{0\le n\le N}$ such that $t^0 = 0$ and $t^N = t_{\rm F}$, together with a set of meshes $\{\mathcal{T}_h^n\}_{0\le n\le N}$. For all $1 \le n \le N$, we define the time interval $I_n := (t^{n-1}, t^n]$ and the time step $\tau^n := t^n - t^{n-1}$. For all $0 \le n \le N$, we assume that $\mathcal{T}_h^n$ covers exactly Ω. The meshes $\mathcal{T}_h^n$ can be composed of general polygonal (polyhedral) elements. For all $T \in \mathcal{T}_h^n$, h_T denotes the diameter of the mesh element T. The discrete times and meshes can be constructed by a space–time adaptive time-marching algorithm such as those of Sections 4.1, 4.3 and 5.1, 5.2, 5.4 below.

Let W be a vector space of functions defined on Ω. We then use the notation $P_\tau^1(W)$ for the vector space of functions v defined on Q such that $v(\cdot, t)$ takes values in W and is continuous and piecewise affine in time. Functions in $P_\tau^1(W)$ are uniquely defined by the $(N+1)$ functions $\{v^n := v(\cdot, t^n)\}_{0\le n\le N}$ in W. Similarly, $P_\tau^0(W)$ denotes the vector space of functions defined on Q such that $v(\cdot, t)$ takes values in W and is piecewise constant in time; for $1 \le n \le N$, we then set $v^n := v(\cdot, t)|_{I_n}$. Functions in $P_\tau^0(W)$ are uniquely defined by the N functions $\{v^n\}_{1\le n\le N}$ in W. Furthermore, we observe that if $v \in P_\tau^1(W)$, then $\partial_t v \in P_\tau^0(W)$ is such that for all $1 \le n \le N$,

$$\partial_t^n v := \partial_t v|_{I_n} = \frac{1}{\tau^n}(v^n - v^{n-1}). \tag{2.2}$$

Finally, let $0 \le n \le N$. We first define the broken Sobolev space $H^1(\mathcal{T}_h^n)$ as the space of such functions $v \in L^2(\Omega)$ that $v|_T \in H^1(T)$ for all $T \in \mathcal{T}_h^n$. The symbol ∇ henceforth denotes the corresponding broken gradient, i.e., a gradient of the function restricted to each mesh element T. Then we also define $P_\tau^1(H^1(\mathcal{T}))$ as the space of functions v continuous and piecewise affine in time, given by $v^n \in H^1(\mathcal{T}_h^n)$ for every discrete time t^n, $0 \le n \le N$, i.e., $\{v^n = v(\cdot, t^n)\}_{0\le n\le N}$ in $H^1(\mathcal{T}_h^n)$.

2.2 Weak solution definition via the global and complementary pressures

In order to characterize the error in an approximate solution to (1.1a)–(1.5b), we first need to define the weak solution of (1.1a)–(1.5b). Solely to this purpose, we, following [17, 5, 18, 19, 20], introduce the global and complementary pressures. We would like to stress that these mathematical quantities only appear in this section in order to describe the weak solution and in Section 2.4 in order to define the error measure, but they are not supposed to be used in the actual numerical treatment.

Let the phase mobilities be denoted by

$$\lambda_\alpha(a) := \frac{k_{{\rm r},\alpha}(a)}{\mu_\alpha} \qquad \alpha \in \{{\rm n}, {\rm w}\}. \tag{2.3}$$

We define the *global pressure*

$$\mathfrak{p}(p_{\rm w}, s_{\rm w}) := p_{\rm w} + \int_0^{s_{\rm w}} \frac{\lambda_{\rm n}(a)}{\lambda_{\rm w}(a) + \lambda_{\rm n}(a)} p_{\rm c}'(a){\rm d}a \tag{2.4}$$

and the *complementary pressure*

$$\mathfrak{q}(s_{\rm w}) := -\int_0^{s_{\rm w}} \frac{\lambda_{\rm w}(a)\lambda_{\rm n}(a)}{\lambda_{\rm w}(a)+\lambda_{\rm n}(a)} p_{\rm c}'(a){\rm d}a. \tag{2.5}$$

Next, in order to simplify the developments below, let us define the functions $\mathbf{v}_\alpha$, $\alpha \in \{{\rm n},{\rm w}\}$, of wetting pressure and saturation $(p_{\rm w}, s_{\rm w})$, by

$$\mathbf{v}_{\rm w}(p_{\rm w}, s_{\rm w}) := -\underline{\mathbf{K}}(\lambda_{\rm w}(s_{\rm w})\nabla\mathfrak{p}(p_{\rm w}, s_{\rm w}) + \nabla\mathfrak{q}(s_{\rm w}) + \lambda_{\rm w}(s_{\rm w})\rho_{\rm w} g\nabla z), \tag{2.6a}$$
$$\mathbf{v}_{\rm n}(p_{\rm w}, s_{\rm w}) := -\underline{\mathbf{K}}(\lambda_{\rm n}(s_{\rm w})\nabla\mathfrak{p}(p_{\rm w}, s_{\rm w}) - \nabla\mathfrak{q}(s_{\rm w}) + \lambda_{\rm n}(s_{\rm w})\rho_{\rm n} g\nabla z). \tag{2.6b}$$

Note that $\mathbf{v}_\alpha(p_{\rm w}, s_{\rm w})$ are formally equivalent to the phase velocities $\mathbf{u}_\alpha$ given by (1.2). We need to introduce the global and complementary pressures $\mathfrak{p}$ and $\mathfrak{q}$ and the functions $\mathbf{v}_{\rm w}(p_{\rm w}, s_{\rm w})$ and $\mathbf{v}_{\rm n}(p_{\rm w}, s_{\rm w})$ as the relations (1.2) may not be properly defined under the regularity assumptions of the weak solution definition, whereas (2.6a)–(2.6b) are always well defined.

We suppose that the data are regular enough so that the weak solution $(p_{\rm w}, s_{\rm w})$ to (1.1a)–(1.5b), setting $s_{\rm n} := 1 - s_{\rm w}$, can be characterized by

$$\partial_t s_{\rm w} \in X',\ \mathfrak{q}(s_{\rm w}) \in X,\ s_{\rm w}(\cdot, 0) = s_{\rm w}^0, \tag{2.7a}$$
$$\mathfrak{p}(p_{\rm w}, s_{\rm w}) \in X, \tag{2.7b}$$
$$(p_{\rm w}(\cdot, t), 1) = 0 \qquad \text{for a.e. } t \in (0, t_{\rm F}), \tag{2.7c}$$
$$\int_0^{t_{\rm F}} \{\langle\partial_t(\phi s_\alpha), \varphi\rangle - (\mathbf{v}_\alpha(p_{\rm w}, s_{\rm w}), \nabla\varphi) - (q_\alpha, \varphi)\}{\rm d}t = 0 \qquad \forall\varphi \in X,\ \alpha \in \{{\rm n},{\rm w}\}. \tag{2.7d}$$

We refer to [18] for the details.

2.3 Approximate saturations and pressures

Our a posteriori error estimates will be given for *general approximate wetting saturations* $s_{{\rm w},h\tau}$ and *general approximate wetting pressures* $p_{{\rm w},h\tau}$, not linked to any particular numerical scheme. More precisely, recalling the definition of the space $P_\tau^1(H^1(\mathcal{T}))$ from Section 2.1, we merely require $s_{{\rm w},h\tau}, p_{{\rm w},h\tau} \in P_\tau^1(H^1(\mathcal{T}))$. Herein, we tacitly assume only lowest-order discretizations in time. In general, the notation $v_{h\tau}$ stands for a space–time function continuous and piecewise affine in time and piecewise polynomial in space on the meshes $\mathcal{T}_h^n$ and $v_h^n := v_{h\tau}(\cdot, t^n)$ for the piecewise polynomial in space. We also assume for simplicity of exposition that $s_{{\rm w},h}^0 = s_{\rm w}^0$ and that $(p_{{\rm w},h\tau}(\cdot, t), 1) = 0$ for all $t \in (0, t_{\rm F})$.

We use the definitions (2.4), (2.5), and (2.6a)–(2.6b) also for the approximate saturations $s_{{\rm w},h\tau}$ and pressures $p_{{\rm w},h\tau}$, i.e., we replace the arguments $s_{\rm w}$ by $s_{{\rm w},h\tau}$ and $p_{\rm w}$ by $p_{{\rm w},h\tau}$. The present framework in particular includes cases where $s_{{\rm w},h\tau}$ and $p_{{\rm w},h\tau}$ are *nonconforming* in the sense that $\mathfrak{q}(s_{{\rm w},h\tau}) \notin X$ and $\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) \notin X$. This happens in particular whenever $\mathfrak{q}(s_{{\rm w},h\tau})$ and $\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau})$ are discontinuous.

2.4 Error measure

The primordial question in a posteriori error estimates is that of the error "measure". In linear problems, one usually chooses the energy norm for a global error measure. In nonlinear problems, the situation is more difficult. One approach consists in taking the dual norm of the residual, i.e., of the difference of the nonlinear operator applied to the exact and approximate solutions, cf. [15, 16, 26, 22]. We also refer to [4, 54, 53] for the use of dual norms in singularly perturbed linear problems. The advantage is that such a measure is dictated by the problem at hand, it simplifies the analysis, and leads to sharper (and possibly robust, as in [26, 22]) estimates.

Let $s_{\rm w}$, $p_{\rm w}$ and $s_{{\rm w},h\tau}$, $p_{{\rm w},h\tau}$ be the exact and approximate wetting saturations and pressures as described in Sections 2.2 and 2.3. Let $s_{\rm n} := 1 - s_{\rm w}$ and $s_{{\rm n},h\tau} := 1 - s_{{\rm w},h\tau}$. We define our error measure by

$$
\begin{aligned}
&|||(s_{\rm w} - s_{{\rm w},h\tau}, p_{\rm w} - p_{{\rm w},h\tau})||| \\
:=& \Bigg\{ \sum_{\alpha\in\{{\rm n},{\rm w}\}} \Bigg\{ \sup_{\varphi\in X,\, \|\varphi\|_X=1} \int_0^{t_{\rm F}} \{\langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle \\
&- (\mathbf{v}_\alpha(p_{\rm w}, s_{\rm w}) - \mathbf{v}_\alpha(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}), \nabla\varphi)\}{\rm d}t \Bigg\}^2 \Bigg\}^{\frac{1}{2}} \\
&+ \left\{ \inf_{\tilde{\mathfrak{p}}\in X} \int_0^{t_{\rm F}} \|\underline{\mathbf{K}}(\lambda_{\rm w}(s_{{\rm w},h\tau}) + \lambda_{\rm n}(s_{{\rm w},h\tau}))\nabla(\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) - \tilde{\mathfrak{p}})\|^2 {\rm d}t \right\}^{\frac{1}{2}} \\
&+ \left\{ \inf_{\tilde{\mathfrak{q}}\in X} \int_0^{t_{\rm F}} \|\underline{\mathbf{K}}\nabla(\mathfrak{q}(s_{{\rm w},h\tau}) - \tilde{\mathfrak{q}})\|^2 {\rm d}t \right\}^{\frac{1}{2}}.
\end{aligned}
\tag{2.8}
$$

For $1 \le n \le N$, a local-in-time version, consisting in replacing in (2.8) the time integral $\int_0^{t_{\rm F}}$ by $\int_{I_n}$ and the space X by $X|_{I_n}$, is denoted by $|||(s_{\rm w} - s_{{\rm w},h\tau}, p_{\rm w} - p_{{\rm w},h\tau})|||_{I_n}$.

The first term of the error measure (2.8) represents the dual norm of the residual. Should $s_{{\rm w},h\tau}$ coincide with $s_{\rm w}$ and $p_{{\rm w},h\tau}$ with $p_{\rm w}$, it equals zero. The second and third terms measure the nonconformity, i.e., the fact that possibly $\mathfrak{q}(s_{{\rm w},h\tau}) \notin X$ and $\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) \notin X$, which is typically the case for mixed finite element, cell-centered finite volume, or discontinuous Galerkin approximations; recall from (2.7a)–(2.7d) that $\mathfrak{q}(s_{\rm w}) \in X$ and $\mathfrak{p}(p_{\rm w}, s_{\rm w}) \in X$ for the exact wetting saturation and pressure. The terms $\underline{\mathbf{K}}(\lambda_{\rm w}(s_{{\rm w},h\tau}) + \lambda_{\rm n}(s_{{\rm w},h\tau}))$ and $\underline{\mathbf{K}}$ in front of the broken gradients represent weights with appropriate physical units and are deduced from the weak formulation, cf. [18, 14]. Shall there hold $\mathfrak{q}(s_{{\rm w},h\tau}) \in X$ and $\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) \in X$, as in the vertex-centered finite volume or finite element method, the second and third terms equal zero.

3 A general a posteriori error estimate

We present here a general a posteriori error estimate giving a guaranteed and fully computable upper bound on the error measure (2.8).

3.1 Pressure and velocities reconstructions

Recall that we merely suppose that the approximate wetting saturation and pressure $s_{{\rm w},h\tau}, p_{{\rm w},h\tau}$ belong to the space $P^1_\tau(H^1(\mathcal{T}))$. In order to proceed generally, without any further specification of the numerical treatment used to obtain $s_{{\rm w},h\tau}, p_{{\rm w},h\tau}$, we now make the following assumption:

Assumption 3.1 (Pressure and velocities reconstructions)**.** *We assume that there exist scalar functions* $\mathfrak{p}_{h\tau}$ *and* $\mathfrak{q}_{h\tau}$ *and vector functions* $\mathbf{u}_{\alpha,h\tau}$*,* $\alpha \in \{{\rm n},{\rm w}\}$*, such that* $\mathfrak{p}_{h\tau}, \mathfrak{q}_{h\tau} \in X$ *and* $\mathbf{u}_{\alpha,h\tau} \in P^0_\tau(\mathbf{H}({\rm div},\Omega))$*,* $\alpha \in \{{\rm n},{\rm w}\}$*. Moreover, we suppose that* $\mathbf{u}_{\alpha,h\tau}$ *satisfy*

$$
(q^n_\alpha - \partial^n_t(\phi s_{\alpha,h\tau}) - \nabla\cdot\mathbf{u}^n_{\alpha,h}, 1)_T = 0 \qquad \forall T \in \mathcal{T}^n_h, \quad \forall 1 \le n \le N, \quad \alpha \in \{{\rm n},{\rm w}\}. \tag{3.1}
$$

We will call $\mathfrak{p}_{h\tau}$ *the* global pressure reconstruction*,* $\mathfrak{q}_{h\tau}$ *the* complementary pressure reconstruction*, and* $\mathbf{u}_{\alpha,h\tau}$*,* $\alpha \in \{{\rm n},{\rm w}\}$*, the* phase velocities reconstructions*.*

Remark 3.2 (Pressure and velocities reconstructions)**.** *In the continuous setting, the global pressure* $\mathfrak{p}(p_{\rm w}, s_{\rm w})$ *and the complementary pressure* $\mathfrak{q}(s_{\rm w})$ *belong to the space* X*, see* (2.7a)–(2.7b)*, which in particular expresses their appropriate continuity. Similarly, it is physical that the normal traces of the phase velocities* $\mathbf{v}_\alpha(p_{\rm w}, s_{\rm w})$ $(\mathbf{u}_\alpha)$*,* $\alpha \in \{{\rm n}, {\rm w}\}$*, are continuous and that the equilibrium condition*

$$\partial_t(\phi s_\alpha) + \nabla\cdot\mathbf{u}_\alpha = q_\alpha \tag{3.2}$$

holds, cf. (1.1a) *and* (1.2)*, which expresses the mass balance and local conservativity for the phase fluxes. These properties are not necessarily satisfied at the discrete level, in the sense that there can hold* $\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) \notin X$*,* $\mathfrak{q}(s_{{\rm w},h\tau}) \notin X$*, and that* $\mathbf{v}_\alpha(p_{{\rm w},h\tau}, s_{{\rm w},h\tau})$*,* $\alpha \in \{{\rm n}, {\rm w}\}$*, are not in equilibrium and their normal traces are discontinuous. The pressure reconstructions* $\mathfrak{p}_{h\tau}, \mathfrak{q}_{h\tau}$ *and the velocity reconstructions* $\mathbf{u}_{\alpha,h\tau}$*,* $\alpha \in \{{\rm n}, {\rm w}\}$ *of Assumption 3.1, restore the properties of the continuous level at the discrete one.*

3.2 A posteriori error estimate

We are now ready to describe our estimators. Let a time step n, $1 \le n \le N$, and a mesh element $T \in \mathcal{T}_h^n$ be given. Recall first the Poincaré inequality:

$$\|\varphi - \varphi_T\|_T \le C_{{\rm P},T} h_T \|\nabla\varphi\|_T \qquad \forall \varphi \in H^1(T), \tag{3.3}$$

where φ_T is the mean value of the function φ on the element T and $C_{{\rm P},T} = 1/\pi$ whenever the element T is convex [47, 8]. Define the *residual estimators*

$$\eta^n_{{\rm R},T,\alpha} := C_{{\rm P},T} h_T \|q^n_\alpha - \partial^n_t(\phi s_{\alpha,h\tau}) - \nabla\cdot\mathbf{u}^n_{\alpha,h}\|_T, \qquad \alpha \in \{{\rm n}, {\rm w}\}, \tag{3.4}$$

the *diffusive flux estimators*

$$\eta^n_{{\rm DF},T,\alpha}(t) := \|\mathbf{u}^n_{\alpha,h} - \mathbf{v}_\alpha(p_{{\rm w},h\tau}, s_{{\rm w},h\tau})(t)\|_T, \qquad \alpha \in \{{\rm n}, {\rm w}\}, \tag{3.5}$$

and the *nonconformity estimators*

$$\eta^n_{{\rm NC},T,1}(t) := \|\underline{\mathbf{K}}(\lambda_{\rm w}(s_{{\rm w},h\tau}) + \lambda_{\rm n}(s_{{\rm w},h\tau}))\nabla(\mathfrak{p}(p_{{\rm w},h\tau}, s_{{\rm w},h\tau}) - \mathfrak{p}_{h\tau})\|_T(t), \tag{3.6a}$$

$$\eta^n_{{\rm NC},T,2}(t) := \|\underline{\mathbf{K}}\nabla(\mathfrak{q}(s_{{\rm w},h\tau}) - \mathfrak{q}_{h\tau})\|_T(t). \tag{3.6b}$$

We then have the following result:

Theorem 3.3 (A posteriori estimate of the overall error)**.** *Let* $(p_{\rm w}, s_{\rm w})$ *be the weak wetting pressure and saturation characterized by* (2.7a)–(2.7d)*. Let* $(s_{{\rm w},h\tau}, p_{{\rm w},h\tau}) \in [P^1_\tau(H^1(\mathcal{T}))]^2$ *be the approximate wetting pressure and saturation. Let the pressure and velocities reconstructions* $\mathfrak{p}_{h\tau}$*,* $\mathfrak{q}_{h\tau}$*, and* $\mathbf{u}_{\alpha,h\tau}$*,* $\alpha \in \{{\rm n}, {\rm w}\}$*, satisfy Assumption 3.1. Let the estimators be given by* (3.4)–(3.6b)*. Then*

$$\begin{aligned}
|||(s_{\rm w} - s_{{\rm w},h\tau}, p_{\rm w} - p_{{\rm w},h\tau})||| \le{}& \left\{\sum_{\alpha\in\{{\rm n},{\rm w}\}} \sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta^n_{{\rm R},T,\alpha} + \eta^n_{{\rm DF},T,\alpha}(t))^2 \,{\rm d}t\right\}^{\frac12} \\
&+ \left\{\sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta^n_{{\rm NC},T,1}(t))^2 \,{\rm d}t\right\}^{\frac12} \\
&+ \left\{\sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta^n_{{\rm NC},T,2}(t))^2 \,{\rm d}t\right\}^{\frac12}.
\end{aligned} \tag{3.7}$$

Proof. The proof is straightforward using the definition of the error measure (2.8) and using Assumption 3.1. The second and third terms in (3.7) clearly issue from the second and third terms on the right hand-side of (2.8). We thus only have to prove that the first term is an upper bound on the first term in the right hand-side of (2.8). Let $\alpha \in \{\mathrm{n}, \mathrm{w}\}$ and $\varphi \in X$, $\|\varphi\|_X = 1$, be given. Then (2.7d) implies that

$$\int_0^{t_{\mathrm{F}}} \{\langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{v}_\alpha(p_{\mathrm{w}}, s_{\mathrm{w}}) - \mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}), \nabla\varphi)\}\mathrm{d}t$$
$$= \int_0^{t_{\mathrm{F}}} \{(q_\alpha - \partial_t(\phi s_{\alpha,h\tau}), \varphi) + \mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}), \nabla\varphi)\}\mathrm{d}t.$$

Let now $1 \le n \le N$ be given. Adding and subtracting $(\mathbf{u}^n_{\alpha,h}, \nabla\varphi)$, using the Green theorem, the assumption (3.1), the Poincaré inequality (3.3), and the Cauchy–Schwarz inequality,

$$\begin{aligned}
&(q^n_\alpha - \partial^n_t(\phi s_{\alpha,h\tau}), \varphi) + (\mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}), \nabla\varphi)\\
&= (q^n_\alpha - \partial^n_t(\phi s_{\alpha,h\tau}) - \nabla\cdot\mathbf{u}^n_{\alpha,h}, \varphi) + (\mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}) - \mathbf{u}^n_{\alpha,h}, \nabla\varphi)\\
&= \sum_{T\in\mathcal{T}^n_h} \{(q^n_\alpha - \partial^n_t(\phi s_{\alpha,h\tau}) - \nabla\cdot\mathbf{u}^n_{\alpha,h}, \varphi - \varphi_T)_T + (\mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}) - \mathbf{u}^n_{\alpha,h}, \nabla\varphi)_T\}\\
&\le \sum_{T\in\mathcal{T}^n_h} \{(\eta^n_{\mathrm{R},T,\alpha} + \eta^n_{\mathrm{DF},T,\alpha}(t))\|\nabla\varphi\|_T\}.
\end{aligned}$$

Thus

$$\sum_{n=1}^N \int_{I_n} \{\langle \partial_t(\phi s_\alpha) - \partial^n_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{v}_\alpha(p_{\mathrm{w}}, s_{\mathrm{w}}) - \mathbf{v}_\alpha(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}), \nabla\varphi)\}\mathrm{d}t$$
$$\le \sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}^n_h} \{(\eta^n_{\mathrm{R},T,\alpha} + \eta^n_{\mathrm{DF},T,\alpha}(t))\|\nabla\varphi\|_T\}\mathrm{d}t,$$

wherefrom the assertion of the theorem follows by the Cauchy–Schwarz inequality and by the fact that $\|\varphi\|_X = 1$. □

3.3 Application to different numerical methods

For the theoretical analysis of this paper, we only need Assumption 3.1. The practical application of the present framework to different numerical methods consists in specifying the construction of $\mathfrak{p}_{h\tau}$, $\mathfrak{q}_{h\tau}$, and $\mathbf{u}_{\alpha,h\tau}$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$ that we outline now.

In vertex-centered finite volume or finite element methods, there typically holds $\mathfrak{p}(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau}) \in X$ and $\mathfrak{q}(s_{\mathrm{w},h\tau}) \in X$, so that we can put $\mathfrak{p}_{h\tau} := \mathfrak{p}(p_{\mathrm{w},h\tau}, s_{\mathrm{w},h\tau})$ and $\mathfrak{q}_{h\tau} := \mathfrak{q}(s_{\mathrm{w},h\tau})$. In the other, nonconforming, numerical methods, we typically choose $\mathfrak{p}_{h\tau} \in P^1_\tau(H^1(\Omega))$, $\mathfrak{p}^n_h := \mathcal{I}_{\mathrm{av}}(\mathfrak{p}(p^n_{\mathrm{w},h}, s^n_{\mathrm{w},h}))$ and $\mathfrak{q}_{h\tau} \in P^1_\tau(H^1(\Omega))$, $\mathfrak{q}^n_h := \mathcal{I}_{\mathrm{av}}(\mathfrak{q}(s^n_{\mathrm{w},h}))$. Here $\mathcal{I}_{\mathrm{av}}$ is the averaging operator which sets the Lagrangian degrees of freedom inside Ω to the average of the values from the different elements sharing this degree of freedom, see [1, 38, 12].

The choice of $\mathbf{u}_{\alpha,h\tau}$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, is more involved. In mixed finite element methods, in addition to the approximate wetting saturation $s_{\mathrm{w},h\tau}$ and pressure $p_{\mathrm{w},h\tau}$ described in Section 2.3, one also directly obtains phase velocity approximations $\mathbf{u}_{\alpha,h\tau} \in P^0_\tau(\mathbf{H}(\mathrm{div}, \Omega))$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, satisfying (3.1). More precisely, for every time interval I_n, $1 \le n \le N$, typically $\mathbf{u}^n_{\alpha,h} \in \mathbf{RTN}(\mathcal{T}^n_h)$, where $\mathbf{RTN}(\mathcal{T}^n_h)$ is the Raviart–Thomas finite-dimensional subspace of $\mathbf{H}(\mathrm{div}, \Omega)$, cf. [10]. In other numerical methods, obtaining $\mathbf{u}_{\alpha,h\tau} \in P_\tau^0(\mathbf{H}(\mathrm{div},\Omega))$ satisfying (3.1) is possible by means of local postprocessing. In the context of linear elliptic equations, we refer for cell-centered finite volume methods to [33, 56], for discontinuous Galerkin methods to [30, 39, 2], and for vertex-centered finite volume and finite element methods to [43, 55]. For nonlinear elliptic equations, such constructions are unified for different numerical methods in [32]. In the context of two-phase flows, the constructions of $\mathbf{u}_{\alpha,h\tau}$, $\alpha \in \{\mathrm{n},\mathrm{w}\}$, can be found in [21] for cell-centered finite volume methods, in [14] for vertex-centered finite volume methods, and in [28, 29] for the discontinuous Galerkin method.

In presence of additional errors stemming from (purposely) not converged linear and nonlinear solvers or iterative coupling, (3.1) does not hold true for the directly available or simply locally reconstructed $\mathbf{u}_{\alpha,h\tau}$. We will give below in Sections 4 and 5 general recipes how to construct $\mathbf{u}_{\alpha,h\tau}$ satisfying (3.1) in such situations. These abstract recipes are illustrated on particular examples in [21, 14].

4 Stopping criteria and adaptivity for fully implicit discretizations

We show in this section how the abstract a posteriori error estimate of Section 3 can be adopted to fully implicit discretizations of (1.1a)–(1.5b). We also show how one can take into account the additional error from iterative linearization and iterative solution of algebraic linear systems and distinguish the different error contributions. We finally propose stopping criteria for the various iterations and design a fully adaptive algorithm.

4.1 A fully implicit formulation

Keeping p_w and s_w as unknowns and expressing s_n as a function of s_w from (1.1b) and p_n as a function of p_w and s_w from (1.1c), we arrive at the following equivalent form of (1.1a)–(1.1c):

$$\partial_t(\phi s_\mathrm{w}) - \nabla\cdot\left(\frac{k_{\mathrm{r,w}}(s_\mathrm{w})}{\mu_\mathrm{w}}\underline{\mathbf{K}}(\nabla p_\mathrm{w} + \rho_\mathrm{w} g\nabla z)\right) = q_\mathrm{w} \qquad \text{in } Q, \tag{4.1a}$$

$$-\partial_t(\phi s_\mathrm{w}) - \nabla\cdot\left(\frac{k_{\mathrm{r,n}}(s_\mathrm{w})}{\mu_\mathrm{n}}\underline{\mathbf{K}}(\nabla(p_\mathrm{w} + p_\mathrm{c}(s_\mathrm{w})) + \rho_\mathrm{n} g\nabla z)\right) = q_\mathrm{n} \qquad \text{in } Q. \tag{4.1b}$$

Let us now suppose some discretization of the above system in both space and time, starting from $s_{\mathrm{w},h}^0 \in H^1(\mathcal{T}_h^0)$. We suppose implicit (backward Euler) discretization in time. This leads, on a time level n, $1 \le n \le N$, to a system of nonlinear algebraic equations that can be schematically written in the form

$$\begin{pmatrix} \mathbb{SS}_\mathrm{w}^n & \mathbb{SP}_\mathrm{w}^n \\ \mathbb{SS}_\mathrm{n}^n & \mathbb{SP}_\mathrm{n}^n \end{pmatrix}\begin{pmatrix} S_\mathrm{w}^n \\ P_\mathrm{w}^n \end{pmatrix} = \begin{pmatrix} D_\mathrm{w}^n \\ D_\mathrm{n}^n \end{pmatrix}, \tag{4.2}$$

where S_w^n is the algebraic vector of discrete unknowns corresponding to the wetting saturation $s_{\mathrm{w},h}^n$ and P_w^n is the algebraic vector of discrete unknowns corresponding to the wetting pressure $p_{\mathrm{w},h}^n$. For the sake of simplicity of the exposition, we suppose herein that there is one unknown per each element of the mesh $\mathcal{T}_h^n$ in both S_w^n and P_w^n. The adaptation to the general case is easy. Note that $\mathbb{SS}_\mathrm{w}^n$, $\mathbb{SP}_\mathrm{w}^n$, $\mathbb{SS}_\mathrm{n}^n$, and $\mathbb{SP}_\mathrm{n}^n$ in (4.2) are nonlinear vector functions and not matrices. In practice, (4.2) is solved using some iterative linearization, typically the Newton–Raphson or the fixed-point ones, where the arising linear systems are solved by some iterative method. This leads to the following algorithm, where we already prepare a path for the application of our a posteriori error estimates:

1. Let the initial wetting saturation S_w^0 (and pressure P_w^0) be given. Set $n = 1$.

2. Set up the system of nonlinear algebraic equations (4.2).

3. (a) Choose some initial wetting saturation $S_{\rm w}^{n,0}$ and pressure $P_{\rm w}^{n,0}$. Typically, these are the saturation and pressure from the last time step, $S_{\rm w}^{n-1}$ and $P_{\rm w}^{n-1}$. Set $k = 1$.

   (b) Set up the following linear system: find $S_{\rm w}^{n,k}$ and $P_{\rm w}^{n,k}$, the solutions to

$$\begin{pmatrix} \mathbb{SS}_{\rm w}^{n,k-1} & \mathbb{SP}_{\rm w}^{n,k-1} \\ \mathbb{SS}_{\rm n}^{n,k-1} & \mathbb{SP}_{\rm n}^{n,k-1} \end{pmatrix} \begin{pmatrix} S_{\rm w}^{n,k} \\ P_{\rm w}^{n,k} \end{pmatrix} = \begin{pmatrix} D_{\rm w}^{n,k-1} \\ D_{\rm n}^{n,k-1} \end{pmatrix}. \tag{4.3}$$

   Here $\mathbb{SS}_{\rm w}^{n,k-1}$, $\mathbb{SP}_{\rm w}^{n,k-1}$, $\mathbb{SS}_{\rm n}^{n,k-1}$, and $\mathbb{SP}_{\rm n}^{n,k-1}$ are matrices formed from $S_{\rm w}^{n,k-1}$ and $P_{\rm w}^{n,k-1}$ and $D_{\rm w}^{n,k-1}$ and $D_{\rm n}^{n,k-1}$ are vectors formed from $S_{\rm w}^{n,k-1}$ and $P_{\rm w}^{n,k-1}$.

   (c) i. Choose some initial saturation $S_{\rm w}^{n,k,0}$ and pressure $P_{\rm w}^{n,k,0}$. Typically, $S_{\rm w}^{n,k,0} = S_{\rm w}^{n,k-1}$ and $P_{\rm w}^{n,k,0} = P_{\rm w}^{n,k-1}$. Set $i = 1$.

   ii. Perform a step of a chosen iterative algebraic method for the solution of the linear system (4.3), starting from $S_{\rm w}^{n,k,i-1}$ and $P_{\rm w}^{n,k,i-1}$. This gives approximations $S_{\rm w}^{n,k,i}$ and $P_{\rm w}^{n,k,i}$.

   iii. Build the discrete functions representations of the wetting saturations and pressures $s_{{\rm w},h}^{n,k,i} \in H^1(\mathcal{T}_h^n)$ and $p_{{\rm w},h}^{n,k,i} \in H^1(\mathcal{T}_h^n)$ from $S_{\rm w}^{n,k,i}$ and $P_{\rm w}^{n,k,i}$, according to the given numerical method. Define the space–time functions $s_{{\rm w},h\tau}^{n,k,i}$ and $p_{{\rm w},h\tau}^{n,k,i}$; these are affine in time on the time interval I_n, given by $s_{{\rm w},h}^{n-1}$ and $p_{{\rm w},h}^{n-1}$ at time t^{n-1} and by $s_{{\rm w},h}^{n,k,i}$ and $p_{{\rm w},h}^{n,k,i}$ at time t^n. We use this refined notation in place of $s_{{\rm w},h\tau}, p_{{\rm w},h\tau}$ of Section 2.3.

   iv. From $s_{{\rm w},h}^{n,k,i}$ and $p_{{\rm w},h}^{n,k,i}$, set $\mathfrak{p}_h^{n,k,i} := \mathcal{I}_{\rm av}(\mathfrak{p}(p_{{\rm w},h}^{n,k,i}, s_{{\rm w},h}^{n,k,i}))$ and $\mathfrak{q}_h^{n,k,i} := \mathcal{I}_{\rm av}(\mathfrak{q}(s_{{\rm w},h}^{n,k,i}))$. Define the global pressure reconstruction $\mathfrak{p}_{h\tau}^{n,k,i}$ and the complementary pressure reconstruction $\mathfrak{q}_{h\tau}^{n,k,i}$ (cf. Assumption 3.1) affine in time on the time interval I_n by $\mathfrak{p}_h^{n-1}$ and $\mathfrak{q}_h^{n-1}$ at time t^{n-1} and by $\mathfrak{p}_h^{n,k,i}$ and $\mathfrak{q}_h^{n,k,i}$ at time t^n.

   v. From the given numerical scheme, build the phase velocities reconstructions $\mathbf{u}_{\alpha,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{T}_h^n)$, $\alpha \in \{{\rm n},{\rm w}\}$ (cf. Assumption 3.1). More precisely, the goal is to obtain the decompositions, $\alpha \in \{{\rm n},{\rm w}\}$,

$$\mathbf{u}_{\alpha,h}^{n,k,i} = \mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i} + \mathbf{a}_{\alpha,h}^{n,k,i}, \tag{4.4a}$$

$$\mathbf{d}_{\alpha,h}^{n,k,i}, \mathbf{l}_{\alpha,h}^{n,k,i}, \mathbf{a}_{\alpha,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{T}_h^n). \tag{4.4b}$$

   Herein, $\mathbf{a}_{\alpha,h}^{n,k,i}$ will be used to monitor the error in the solution of the linear algebraic system (4.3), $\mathbf{l}_{\alpha,h}^{n,k,i}$ will be used to monitor the error in the linearization of (4.2) by (4.3), and $\mathbf{d}_{\alpha,h}^{n,k,i}$ will be used to monitor the discretization error. Structurally, this can be achieved as follows:

   A. From the given numerical method, reconstruct locally $\mathbf{d}_{\alpha,h}^{n,k,i}$, $\alpha \in \{{\rm n},{\rm w}\}$, see the discussion in Section 3.3. Typically, the degrees of freedom of $\mathbf{d}_{\alpha,h}^{n,k,i}$ are prescribed using the available functions $\mathbf{v}_\alpha(p_{{\rm w},h}^{n,k,i}, s_{{\rm w},h}^{n,k,i})$; in any case, this construction should be independent of the linearization used to obtain (4.3) and of the iterative algebraic solver used to solve (4.3).

   B. From $S_{\rm w}^{n,k,i}$ and $P_{\rm w}^{n,k,i}$, compute the algebraic residual vectors $R_{\rm w}^{n,k,i}$ and $R_{\rm n}^{n,k,i}$ of (4.3):

$$\begin{pmatrix} R_{\rm w}^{n,k,i} \\ R_{\rm n}^{n,k,i} \end{pmatrix} := -\begin{pmatrix} \mathbb{SS}_{\rm w}^{n,k-1} & \mathbb{SP}_{\rm w}^{n,k-1} \\ \mathbb{SS}_{\rm n}^{n,k-1} & \mathbb{SP}_{\rm n}^{n,k-1} \end{pmatrix} \begin{pmatrix} S_{\rm w}^{n,k,i} \\ P_{\rm w}^{n,k,i} \end{pmatrix} + \begin{pmatrix} D_{\rm w}^{n,k-1} \\ D_{\rm n}^{n,k-1} \end{pmatrix}. \tag{4.5}$$

C. From the given numerical method, define implicitly $\mathbf{l}_{\alpha,h}^{n,k,i}$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, such that

$$(q_\alpha^n - \partial_t^n(\phi s_{\alpha,h\tau}^{n,k,i}) - \nabla\cdot(\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}), 1)_T = R_\alpha^{n,k,i}|_T \qquad \forall T \in \mathcal{T}_h^n, \quad \alpha \in \{\mathrm{n}, \mathrm{w}\}. \tag{4.6}$$

It is crucial to ensure that $\|\mathbf{l}_{\alpha,h}^{n,k,i}\|$ go to zero when $S_{\mathrm{w}}^{n,k}, P_{\mathrm{w}}^{n,k}$, the solutions of (4.3), converge to $S_{\mathrm{w}}^n, P_{\mathrm{w}}^n$, the solution of (4.2).

D. Construct locally $\mathbf{a}_{\alpha,h}^{n,k,i}$, $\alpha \in \{\mathrm{n}, \mathrm{w}\}$, such that

$$(\nabla\cdot\mathbf{a}_{\alpha,h}^{n,k,i}, 1)_T = R_\alpha^{n,k,i}|_T \qquad \forall T \in \mathcal{T}_h^n, \quad \alpha \in \{\mathrm{n}, \mathrm{w}\}, \tag{4.7}$$

using, for instance, the algorithm of [37, Section 7.3], see also [32]. It is crucial to ensure that $\|\mathbf{a}_{\alpha,h}^{n,k,i}\|$ go to zero when $R_\alpha^{n,k,i}$ go to zero.

vi. Check the convergence criterion for the linear solver (see (4.15) below); if this criterion is reached, set $S_{\mathrm{w}}^{n,k} := S_{\mathrm{w}}^{n,k,i}$ and $P_{\mathrm{w}}^{n,k} := P_{\mathrm{w}}^{n,k,i}$. If not, set $i := i+1$ and go back to step 3(c)ii.

(d) Check the convergence criterion for the nonlinear solver (see (4.16) below); if this criterion is reached, set $S_{\mathrm{w}}^n := S_{\mathrm{w}}^{n,k}, P_{\mathrm{w}}^n := P_{\mathrm{w}}^{n,k}$ and $\mathfrak{p}_h^n := \mathfrak{p}_h^{n,k,i}, \mathfrak{q}_h^n := \mathfrak{q}_h^{n,k,i}$. If not, $k := k+1$ and go back to step 3b.

4. Check whether the spatial and temporal errors are comparable (see (4.17a) below), whether the spatial errors are equally distributed in the computational domain (see (4.17b) below), and whether the total error is small enough (see (4.17c) below); if this is the case, set $n := n+1$ and go to step 2. If not, refine the time step τ^n and/or the space mesh $\mathcal{T}_h^n$ and go to step 2.

4.2 An a posteriori error estimate distinguishing the space, time, linearization, and algebraic errors

We now further develop the framework of Section 3 in order to distinguish the space, time, linearization, and algebraic errors.

Fix $\alpha \in \{\mathrm{n}, \mathrm{w}\}$ and consider the algorithm of Section 4.1 on the time step n, linearization step k, and algebraic solver step i. Observe from (4.4a), (4.6), and (4.7) that $\mathbf{u}_{\alpha,h}^{n,k,i}$ satisfies

$$(q_\alpha^n - \partial_t^n(\phi s_{\alpha,h\tau}^{n,k,i}) - \nabla\cdot\mathbf{u}_{\alpha,h}^{n,k,i}, 1)_T = 0 \qquad \forall T \in \mathcal{T}_h^n, \tag{4.8}$$

i.e., $\mathbf{u}_{\alpha,h}^{n,k,i}$ satisfies assumption (3.1). Rewriting (3.4)–(3.6b) with these notations, we pose, for $T \in \mathcal{T}_h^n$,

$$\eta_{\mathrm{R},T,\alpha}^{n,k,i} := C_{\mathrm{P},T} h_T \|q_\alpha^n - \partial_t^n(\phi s_{\alpha,h\tau}^{n,k,i}) - \nabla\cdot\mathbf{u}_{\alpha,h}^{n,k,i}\|_T, \tag{4.9a}$$

$$\eta_{\mathrm{DF},T,\alpha}^{n,k,i}(t) := \|\mathbf{u}_{\alpha,h}^{n,k,i} - \mathbf{v}_\alpha(p_{\mathrm{w},h\tau}^{n,k,i}, s_{\mathrm{w},h\tau}^{n,k,i})(t)\|_T, \tag{4.9b}$$

$$\eta_{\mathrm{NC},T,1}^{n,k,i}(t) := \|\underline{\mathbf{K}}(\lambda_{\mathrm{w}}(s_{\mathrm{w},h\tau}^{n,k,i}) + \lambda_{\mathrm{n}}(s_{\mathrm{w},h\tau}^{n,k,i}))\nabla(\mathfrak{p}(p_{\mathrm{w},h\tau}^{n,k,i}, s_{\mathrm{w},h\tau}^{n,k,i}) - \mathfrak{p}_{h\tau}^{n,k,i})\|_T(t), \tag{4.9c}$$

$$\eta_{\mathrm{NC},T,2}^{n,k,i}(t) := \|\underline{\mathbf{K}}\nabla(\mathfrak{q}(s_{\mathrm{w},h\tau}^{n,k,i}) - \mathfrak{q}_{h\tau}^{n,k,i})\|_T(t). \tag{4.9d}$$

We then have, as in Section 3.2, the local-in-time iterative-algorithms-running version of Theorem 3.3:

Corollary 4.1 (Local-in-time estimate for linearization and algebraic iterates)**.** *Let* $(p_{\mathrm{w}}, s_{\mathrm{w}})$ *be the weak wetting pressure and saturation characterized by* (2.7a)–(2.7d)*. Consider the* n*-th time step,* k*-th linearization step, and* i*-th algebraic solver step of the algorithm of Section 4.1. Let* $s_{\mathrm{w},h\tau}^{n,k,i}$ *and* $p_{\mathrm{w},h\tau}^{n,k,i}$*,* $\mathfrak{p}_{h\tau}^{n,k,i}$ *and* $\mathfrak{q}_{h\tau}^{n,k,i}$*, and* $\mathbf{u}_{\alpha,h}^{n,k,i}$ *be as specified in Section 4.1. Let the estimators be given by* (4.9a)–(4.9d)*. Then*

$$|||(s_{\mathrm{w}} - s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w}} - p_{\mathrm{w},h\tau}^{n,k,i})|||_{I_n} \leq \eta^n := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{R},T,\alpha}^{n,k,i} + \eta_{\mathrm{DF},T,\alpha}^{n,k,i}(t))^2 \,\mathrm{dt} \right\}^{\frac{1}{2}}$$
$$+ \left\{ \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{NC},T,1}^{n,k,i}(t))^2 \,\mathrm{dt} \right\}^{\frac{1}{2}} + \left\{ \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{NC},T,2}^{n,k,i}(t))^2 \,\mathrm{dt} \right\}^{\frac{1}{2}}.$$

We now distinguish the different error components. Define the *spatial estimator*

$$\eta_{\mathrm{sp},T}^{n,k,i}(t) := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \left(\eta_{\mathrm{R},T,\alpha}^{n,k,i} + \|\mathbf{d}_{\alpha,h}^{n,k,i} - \mathbf{v}_\alpha(p_{\mathrm{w},h}^{n,k,i}, s_{\mathrm{w},h}^{n,k,i})\|_T\right)^2 + \left(\eta_{\mathrm{NC},T,1}^{n,k,i}(t)\right)^2 + \left(\eta_{\mathrm{NC},T,2}^{n,k,i}(t)\right)^2 \right\}^{\frac{1}{2}}, \tag{4.10}$$

the *temporal estimators*

$$\eta_{\mathrm{tm},T,\alpha}^{n,k,i}(t) := \|\mathbf{v}_\alpha(p_{\mathrm{w},h\tau}^{n,k,i}, s_{\mathrm{w},h\tau}^{n,k,i})(t) - \mathbf{v}_\alpha(p_{\mathrm{w},h}^{n,k,i}, s_{\mathrm{w},h}^{n,k,i})\|_T, \qquad \alpha \in \{\mathrm{n},\mathrm{w}\}, \tag{4.11}$$

the *linearization estimators*

$$\eta_{\mathrm{lin},T,\alpha}^{n,k,i} := \|\mathbf{l}_{\alpha,h}^{n,k,i}\|_T, \qquad \alpha \in \{\mathrm{n},\mathrm{w}\}, \tag{4.12}$$

and the *algebraic estimators*

$$\eta_{\mathrm{alg},T,\alpha}^{n,k,i} := \|\mathbf{a}_{\alpha,h}^{n,k,i}\|_T, \qquad \alpha \in \{\mathrm{n},\mathrm{w}\}. \tag{4.13}$$

Define also global versions of these estimators as

$$\eta_{\mathrm{sp}}^{n,k,i} := \left\{ 3 \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{sp},T}^{n,k,i}(t))^2 \,\mathrm{dt} \right\}^{\frac{1}{2}}, \tag{4.14a}$$

$$\eta_{\mathrm{tm}}^{n,k,i} := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \int_{I_n} \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{tm},T,\alpha}^{n,k,i}(t))^2 \,\mathrm{dt} \right\}^{\frac{1}{2}}, \tag{4.14b}$$

$$\eta_{\mathrm{lin}}^{n,k,i} := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \tau^n \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{lin},T,\alpha}^{n,k,i})^2 \right\}^{\frac{1}{2}}, \tag{4.14c}$$

$$\eta_{\mathrm{alg}}^{n,k,i} := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \tau^n \sum_{T\in\mathcal{T}_h^n} (\eta_{\mathrm{alg},T,\alpha}^{n,k,i})^2 \right\}^{\frac{1}{2}}. \tag{4.14d}$$

Corollary 4.1 and the triangle inequality yield:

Corollary 4.2 (An a posteriori error estimate distinguishing the space, time, linearization, and algebraic errors)**.** *Let the assumptions of Corollary 4.1 be satisfied. Let the estimators be given by* (4.14a)–(4.14d)*. Then*

$$|||(s_{\rm w}-s_{{\rm w},h\tau}^{n,k,i},p_{\rm w}-p_{{\rm w},h\tau}^{n,k,i})|||_{I_n}\le\eta_{\rm sp}^{n,k,i}+\eta_{\rm tm}^{n,k,i}+\eta_{\rm lin}^{n,k,i}+\eta_{\rm alg}^{n,k,i}.$$

Remark 4.3 (Comments on the different estimators)**.** *The spatial estimators $\eta_{{\rm sp},T}^{n,k,i}$ above regroup all the parts of the estimates of Corollary 4.1 that represent the error in space, typically because the spatial mesh $\mathcal{T}_h^n$ is not fine enough. The temporal estimators $\eta_{{\rm tm},T,\alpha}^{n,k,i}$ represent the part of the error in time, caused by a too big time step τ^n. The linearization estimators $\eta_{{\rm lin},T,\alpha}^{n,k,i}$ measure the error in the linearization* (4.3) *of* (4.2) *on step k. Finally, the algebraic estimators $\eta_{{\rm alg},T,\alpha}^{n,k,i}$ measure the error on the i-th step iterative solution of the linear system* (4.3)*.*

4.3 Stopping criteria and optimal balancing of the different error components

We precise here the algorithm of Section 4.1, in the purpose to balance the error components of Corollary 4.2.

On step 3(c)vi of the algorithm of Section 4.1, we evaluate all $\eta_{\rm sp}^{n,k,i}$, $\eta_{\rm tm}^{n,k,i}$, $\eta_{\rm lin}^{n,k,i}$, and $\eta_{\rm alg}^{n,k,i}$. Then the stopping criterion for the iterative solution of the linear system (4.3) is

$$\eta_{\rm alg}^{n,k,i}\le\gamma_{\rm alg}(\eta_{\rm sp}^{n,k,i}+\eta_{\rm tm}^{n,k,i}+\eta_{\rm lin}^{n,k,i}).\tag{4.15}$$

Here $0<\gamma_{\rm alg}\le 1$ is a user-given weight, typically close to 1. Criterion (4.15) expresses that there is no need to continue with the linear solver iterations if the overall error is dominated by the other components.

Similarly, on step 3d of the algorithm of Section 4.1, we evaluate $\eta_{\rm sp}^{n,k,i}$, $\eta_{\rm tm}^{n,k,i}$, and $\eta_{\rm lin}^{n,k,i}$ and stop the iterative linearization of (4.2) whenever

$$\eta_{\rm lin}^{n,k,i}\le\gamma_{\rm lin}(\eta_{\rm sp}^{n,k,i}+\eta_{\rm tm}^{n,k,i}).\tag{4.16}$$

Here $0<\gamma_{\rm lin}\le 1$ is a user-given weight, typically close to 1. Criterion (4.16) expresses that there is no need to continue with the linearization iterations if the overall error is dominated by the other components.

Finally, on step 4 of the algorithm of Section 4.1, we evaluate $\eta_{\rm sp}^{n,k,i}$, $\eta_{\rm tm}^{n,k,i}$, and $\eta_{{\rm sp},T}^{n,k,i}$ for all $T\in\mathcal{T}_h^n$. The purpose is to achieve

$$\eta_{\rm sp}^{n,k,i}\approx\eta_{\rm tm}^{n,k,i},\tag{4.17a}$$

$$\left\{\int_{I_n}(\eta_{{\rm sp},T}^{n,k,i}(t))^2\,{\rm d}t\right\}^{\frac12}\text{are comparable for all } T\in\mathcal{T}_h^n,\tag{4.17b}$$

$$\eta^n\le\varepsilon^n.\tag{4.17c}$$

Here ε^n is a user-given criterion for the maximal error allowed on the time interval I_n.

Remark 4.4 (Local stopping criteria)**.** *Following [37], [26], and [32], versions of* (4.15) *and* (4.16) *localized on the elements of the mesh $\mathcal{T}_h^n$ can also be given and should be used whenever one intends to refine the space meshes $\mathcal{T}_h^n$ adaptively according to* (4.17b)*.*

Remark 4.5 (Evaluation cost)**.** *The evaluation of the different estimators of Corollaries 4.1 and 4.2 and of the stopping criteria* (4.15)–(4.17c) *has linear cost in terms of the number of the elements of the meshes $\mathcal{T}_h^n$. Moreover, it can be done completely in parallel. In practice, various computational simplifications or approximations may be devised and in order to still reduce the cost, the estimators and stopping criteria need not to be evaluated on every iteration but only on every couple of iterations.*

5 Stopping criteria and adaptivity for implicit pressure–explicit saturations-type discretizations

We give here our a posteriori error estimates and adaptive linear solver and iterative coupling stopping criteria suitable for implicit pressure–explicit saturations-type discretizations.

5.1 Iterative coupling for the pressure–saturation formulation

We first proceed as in Section 4 to obtain (4.1a)–(4.1b). We keep the wetting phase saturation equation (4.1a), whereas we replace the nonwetting phase saturation equation (4.1b) by the sum of (4.1a) and (4.1b). We thus arrive at the following equivalent "pressure–saturation" formulation of (1.1a)–(1.1c):

$$-\nabla\cdot\left(\left(\frac{k_{\mathrm{r,w}}(s_{\mathrm{w}})}{\mu_{\mathrm{w}}}+\frac{k_{\mathrm{r,n}}(s_{\mathrm{w}})}{\mu_{\mathrm{n}}}\right)\underline{\mathbf{K}}\nabla p_{\mathrm{w}} + \frac{k_{\mathrm{r,n}}(s_{\mathrm{w}})}{\mu_{\mathrm{n}}}\underline{\mathbf{K}}(\nabla p_{\mathrm{c}}(s_{\mathrm{w}})+\rho_{\mathrm{n}} g\nabla z)+\frac{k_{\mathrm{r,w}}(s_{\mathrm{w}})}{\mu_{\mathrm{w}}}\underline{\mathbf{K}}\rho_{\mathrm{w}} g\nabla z\right) = q_{\mathrm{w}}+q_{\mathrm{n}} \quad \text{in } Q, \tag{5.1a}$$

$$\partial_t(\phi s_{\mathrm{w}}) - \nabla\cdot\left(\frac{k_{\mathrm{r,w}}(s_{\mathrm{w}})}{\mu_{\mathrm{w}}}\underline{\mathbf{K}}(\nabla p_{\mathrm{w}}+\rho_{\mathrm{w}} g\nabla z)\right) = q_{\mathrm{w}} \quad \text{in } Q. \tag{5.1b}$$

This formulation leads to the following solution algorithm:

1. Let the initial wetting saturation $s^0_{\mathrm{w},h} \in H^1(\mathcal{T}^0_h)$ (and pressure $p^0_{\mathrm{w},h} \in H^1(\mathcal{T}^0_h)$) be given. Set $n = 1$.
2. (a) Choose some initial wetting saturation $s^{n,0}_{\mathrm{w},h}$ ($S^{n,0}_{\mathrm{w}}$ is the corresponding algebraic vector). Typically, this is the approximate saturation from the last time step, $s^{n-1}_{\mathrm{w},h}$. Set $k = 1$.

   (b) Set up the following linear elliptic problem, stemming from (5.1a), with p_{w} as the unknown:

$$-\nabla\cdot\left(\left(\frac{k_{\mathrm{r,w}}(s^{n,k-1}_{\mathrm{w},h})}{\mu_{\mathrm{w}}}+\frac{k_{\mathrm{r,n}}(s^{n,k-1}_{\mathrm{w},h})}{\mu_{\mathrm{n}}}\right)\underline{\mathbf{K}}\nabla p_{\mathrm{w}} - \frac{k_{\mathrm{r,n}}(s^{n,k-1}_{\mathrm{w},h})}{\mu_{\mathrm{n}}}\underline{\mathbf{K}}(\nabla p_{\mathrm{c}}(s^{n,k-1}_{\mathrm{w},h})+\rho_{\mathrm{n}} g\nabla z)+\frac{k_{\mathrm{r,w}}(s^{n,k-1}_{\mathrm{w},h})}{\mu_{\mathrm{w}}}\underline{\mathbf{K}}\rho_{\mathrm{w}} g\nabla z\right) = q_{\mathrm{w}}+q_{\mathrm{n}} \quad \text{in } Q. \tag{5.2}$$

   After a spatial discretization, this problem corresponds to, in matrix form,

$$\mathbb{P}^{n,k-1}_{\mathrm{wn}} P^{n,k}_{\mathrm{w}} = D^{n,k-1}_{\mathrm{wn}}, \tag{5.3}$$

   where the matrix $\mathbb{P}^{n,k-1}_{\mathrm{wn}}$ and the right-hand side vector $D^{n,k-1}_{\mathrm{wn}}$ depend on $S^{n,k-1}_{\mathrm{w}}$.

   (c) i. Choose some initial pressure $P^{n,k,0}_{\mathrm{w}}$. Set $i = 1$.

   ii. Perform a step of a chosen iterative algebraic method for the solution of (5.3), starting from $P^{n,k,i-1}_{\mathrm{w}}$. At the present stage, we have approximations $S^{n,k-1}_{\mathrm{w}}$ and $P^{n,k,i}_{\mathrm{w}}$.

   iii. Build the discrete functions representations of the wetting saturations and pressures $s^{n,k-1}_{\mathrm{w},h} \in H^1(\mathcal{T}^n_h)$ and $p^{n,k,i}_{\mathrm{w},h} \in H^1(\mathcal{T}^n_h)$ from $S^{n,k-1}_{\mathrm{w}}$ and $P^{n,k,i}_{\mathrm{w}}$, according to the given numerical method. Define the space–time functions $s^{n,k-1}_{\mathrm{w},h\tau}$ and $p^{n,k,i}_{\mathrm{w},h\tau}$; these are affine in time on the time interval I_n, given by $s^{n-1}_{\mathrm{w},h}$ and $p^{n-1}_{\mathrm{w},h}$ at time t^{n-1} and by $s^{n,k-1}_{\mathrm{w},h}$ and $p^{n,k,i}_{\mathrm{w},h}$ at time t^n.

iv. From $s_{\mathrm{w},h}^{n,k-1}$ and $p_{\mathrm{w},h}^{n,k,i}$, set $\mathfrak{p}_h^{n,k,i} := \mathcal{I}_{\mathrm{av}}(\mathfrak{p}(p_{\mathrm{w},h}^{n,k,i}, s_{\mathrm{w},h}^{n,k-1}))$ and $\mathfrak{q}_h^{n,k-1} := \mathcal{I}_{\mathrm{av}}(\mathfrak{q}(s_{\mathrm{w},h}^{n,k-1}))$. Define the global pressure reconstruction $\mathfrak{p}_{h\tau}^{n,k,i}$ and the complementary pressure reconstruction $\mathfrak{q}_{h\tau}^{n,k-1}$ (cf. Assumption 3.1) affine in time on the time interval I_n by $\mathfrak{p}_h^{n-1}$ and $\mathfrak{q}_h^{n-1}$ at time t^{n-1} and by $\mathfrak{p}_h^{n,k,i}$ and $\mathfrak{q}_h^{n,k-1}$ at time t^n.

v. From the given numerical scheme, build the phase velocities reconstructions $\mathbf{u}_{\alpha,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{T}_h^n)$, $\alpha \in \{\mathrm{n},\mathrm{w}\}$ (cf. Assumption 3.1). More precisely, the goal is to obtain the decompositions (4.4a)–(4.4b), see step 3(c)v of the algorithm of Section 4.1. Here, $\mathbf{a}_{\alpha,h}^{n,k,i}$ monitor the algebraic error in (5.3), $\mathbf{l}_{\alpha,h}^{n,k,i}$ monitor the error in the iterative coupling, and $\mathbf{d}_{\alpha,h}^{n,k,i}$ monitor the discretization error. Structurally, this can be achieved as follows:

A. From the given numerical method, reconstruct locally $\mathbf{d}_{\alpha,h}^{n,k,i}$, $\alpha \in \{\mathrm{n},\mathrm{w}\}$, as in the step 3(c)vA of the algorithm of Section 4.1, using the available functions $\mathbf{v}_\alpha(p_{\mathrm{w},h}^{n,k,i}, s_{\mathrm{w},h}^{n,k-1})$.

B. From $S_{\mathrm{w}}^{n,k-1}$ and $P_{\mathrm{w}}^{n,k,i}$, compute the algebraic residual vector $R_{\mathrm{wn}}^{n,k,i}$:

$$R_{\mathrm{wn}}^{n,k,i} := -\mathbb{P}_{\mathrm{wn}}^{n,k-1} P_{\mathrm{w}}^{n,k,i} + D_{\mathrm{wn}}^{n,k-1}. \tag{5.4}$$

C. From the given method, define implicitly a vector field $\mathbf{l}_{\mathrm{wn},h}^{n,k,i} \in \mathbf{RTN}(\mathcal{T}_h^n)$ such that

$$(q_{\mathrm{w}}^n + q_{\mathrm{n}}^n - \nabla\cdot(\mathbf{d}_{\mathrm{n},h}^{n,k,i} + \mathbf{d}_{\mathrm{w},h}^{n,k,i} + \mathbf{l}_{\mathrm{wn},h}^{n,k,i}), 1)_T = R_{\mathrm{wn}}^{n,k,i}|_T \qquad \forall T \in \mathcal{T}_h^n. \tag{5.5}$$

In contrast to Section 4, where an independent field $\mathbf{l}_{\alpha,h}^{n,k,i}$ is readily obtained for each phase $\alpha \in \{\mathrm{n},\mathrm{w}\}$, we at the present stage only have one vector field $\mathbf{l}_{\mathrm{wn},h}^{n,k,i}$, representing the total "iterative coupling error". In order to obtain $\mathbf{l}_{\alpha,h}^{n,k,i}$, $\alpha \in \{\mathrm{n},\mathrm{w}\}$, we now suppose that $n = 1$ and $k > 1$ or $n \geq 2$ (for $n = 1$ and $k = 1$, we need to first make once the step 2d below). Using also the discretization of the saturation equation (5.7) below, we can split $\mathbf{l}_{\mathrm{wn},h}^{n,k,i}$ into $\mathbf{l}_{\mathrm{wn},h}^{n,k,i} = \mathbf{l}_{\mathrm{w},h}^{n,k,i} + \mathbf{l}_{\mathrm{n},h}^{n,k,i}$.

D. Construct a vector field $\mathbf{a}_{\mathrm{wn}}^{n,k,i} \in \mathbf{RTN}(\mathcal{T}_h^n)$ such that

$$(\nabla\cdot\mathbf{a}_{\mathrm{wn}}^{n,k,i}, 1)_T = R_{\mathrm{wn}}^{n,k,i}|_T \qquad \forall T \in \mathcal{T}_h^n, \tag{5.6}$$

using, for instance, the algorithm of [37, Section 7.3], see also [32]. As above, we need to split $\mathbf{a}_{\mathrm{wn}}^{n,k,i} = \mathbf{a}_{\mathrm{w}}^{n,k,i} + \mathbf{a}_{\mathrm{n}}^{n,k,i}$, using also the discretization of the saturation equation (5.7) below.

vi. Check the convergence criterion for the linear solver (see (4.15)); if the criterion is reached, set $P_{\mathrm{w}}^{n,k} := P_{\mathrm{w}}^{n,k,i}$. If not, set $i := i + 1$ and go back to step 2(c)ii.

(d) Set up the following hyperbolic-like problem, stemming from (5.1b), with $p_{\mathrm{w},h}^{n,k}$ corresponding to $P_{\mathrm{w}}^{n,k}$: find s_{w} such that

$$\partial_t(\phi s_{\mathrm{w}}) - \nabla\cdot\left(\frac{k_{\mathrm{r,w}}(s_{\mathrm{w}})}{\mu_{\mathrm{w}}}\underline{\mathbf{K}}(\nabla p_{\mathrm{w},h}^{n,k} + \rho_{\mathrm{w}} g \nabla z)\right) = q_{\mathrm{w}} \qquad \text{in } Q. \tag{5.7}$$

Discretize (5.7) in space and in time. The temporal discretization is explicit. This gives $S_{\mathrm{w}}^{n,k}$. Build $s_{\mathrm{w},h}^{n,k} \in H^1(\mathcal{T}_h^n)$ and the space–time approximation $s_{\mathrm{w},h\tau}^{n,k}$, given by $s_{\mathrm{w},h}^{n-1}$ at t^{n-1} and by $s_{\mathrm{w},h}^{n,k}$ at t^n. Repeat steps 2(c)iii–2(c)vD with $s_{\mathrm{w},h}^{n,k-1}$ replaced by $s_{\mathrm{w},h}^{n,k}$.

(e) Check the convergence criterion for the iterative coupling (see (4.16)); if this criterion is reached, set $S_{\rm w}^n := S_{\rm w}^{n,k}$, $P_{\rm w}^n := P_{\rm w}^{n,k}$ and $\mathfrak{p}_h^n := \mathfrak{p}_h^{n,k,i}$, $\mathfrak{q}_h^n := \mathfrak{q}_h^{n,k}$. If not, set $k := k+1$ and go back to step 2b.

3. Check whether the spatial and temporal errors are comparable (see (4.17a)), whether the spatial errors are equally distributed in the computational domain (see (4.17b)), and whether the total error is small enough (see (4.17c)); if this is the case, set $n := n+1$ and go to step 2a. If not, refine the time step τ^n and/or the space mesh $\mathcal{T}_h^n$ and go to step 2a.

5.2 Implicit pressure–explicit saturation formulation

Implicit pressure–explicit saturation discretization (IMPES) corresponds to the iterative coupling algorithm of Section 5.1 where only one step in k ($k = 1$ only) is done.

5.3 An a posteriori error estimate distinguishing the space, time, iterative coupling, and algebraic errors

We now use the framework of Section 3, or more precisely that developed in Section 4.2, in order to distinguish the space, time, iterative coupling, and algebraic errors.

Fix $\alpha \in \{{\rm n}, {\rm w}\}$ and consider the algorithm of Section 5.1 on the time step n, iterative coupling step k, and algebraic solver step i. The approximate wetting pressure at our disposal is thus $p_{{\rm w},h\tau}^{n,k,i}$. Suppose next that we have at hand the l-th iterative coupling step saturation approximation $s_{{\rm w},h\tau}^{n,l}$, where $l = k-1$ or $l = k$. That is, we are either on step 2(c)vi, or on step 2e of the algorithm of Section 5.1. Define

$$\mathbf{u}_{{\rm wn},h}^{n,k,i} := \mathbf{d}_{{\rm n},h}^{n,k,i} + \mathbf{d}_{{\rm w},h}^{n,k,i} + \mathbf{l}_{{\rm wn},h}^{n,k,i} + \mathbf{a}_{\rm wn}^{n,k,i}$$

and observe from (5.5) and (5.6) that $\mathbf{u}_{{\rm wn},h}^{n,k,i}$ satisfies

$$(q_{\rm w}^n + q_{\rm n}^n - \nabla{\cdot}\mathbf{u}_{{\rm wn},h}^{n,k,i}, 1)_T = 0 \qquad \forall T \in \mathcal{T}_h^n.$$

Moreover, the decompositions of $\mathbf{l}_{{\rm wn},h}^{n,k,i}$ and $\mathbf{a}_{\rm wn}^{n,k,i}$ of Section 5.1 have to be such that we can recover the individual phases fluxes reconstructions $\mathbf{u}_{\alpha,h}^{n,k,i}$, $\alpha \in \{{\rm n}, {\rm w}\}$, such that $\mathbf{u}_{{\rm wn},h}^{n,k,i} = \mathbf{u}_{{\rm w},h}^{n,k,i} + \mathbf{u}_{{\rm n},h}^{n,k,i}$ and such that (4.8) holds.

Replacing in terminology the "k-th linearization step" by the "k-th iterative coupling step" and $s_{{\rm w},h\tau}^{n,k,i}$ by $s_{{\rm w},h\tau}^{n,l}$, Corollary 4.1 holds true also in this case. Similarly, keeping the definitions (4.10)–(4.14d) ($\eta_{{\rm lin},T,\alpha}^{n,k,i}$ and $\eta_{\rm lin}^{n,k,i}$ rather represent here the *iterative coupling error*), Corollary 4.2 holds true also in this case.

5.4 Stopping criteria and optimal balancing of the different error components

Stopping criteria to be used on steps 2(c)vi, 2e, and 3 of the algorithm of Section 5.1 for optimal balancing of the different error components and overall error control are exactly the same as in Section 4.3.

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