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# A posteriori error estimates and stopping criteria for space-time domain decomposition for two-phase flow between different rock types\*

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## Abstract

We consider two-phase flow in a porous medium composed of two different rock types, so that the capillary pressure field is discontinuous at the interface between the rocks. This is a nonlinear and degenerate parabolic problem with nonlinear and discontinuous transmission conditions on the interface. We first describe a space-time domain decomposition method based on the optimized Schwarz waveform relaxation algorithm (OSWR) with Robin or Ventcell transmission conditions. Complete numerical approximation is achieved by a finite volume scheme in space and the backward Euler scheme in time. We then derive a guaranteed and fully computable a posteriori error estimate which in particular takes into account the domain decomposition error. Precisely, at each iteration of the OSWR algorithm and at each linearization step, the estimate delivers a guaranteed upper bound on the error between the exact and the approximate solution. Furthermore, to make the algorithm efficient, the different error components given by the spatial discretization, the temporal discretization, the linearization, and the domain decomposition are distinguished. These ingredients are then used to design a stopping criterion for the OSWR algorithm as well as for the linearization iterations, which together lead to important computational savings. Numerical experiments illustrate the efficiency of our estimates and the performance of the OSWR algorithm with adaptive stopping criteria on a model problem in three space dimensions. Additionally, the results show how a posteriori error estimates can help determine the free Robin or Ventcell parameters.

**Key words:** two-phase Darcy flow, discontinuous capillary pressure, finite volume scheme, domain decomposition method, optimized Schwarz waveform relaxation, Robin and Ventcell transmission conditions, linearization, a posteriori error estimate, stopping criteria

## 1 Introduction

Two-phase flows in porous media are of interest in many applications, such as CO<sub>2</sub> sequestration in saline aquifers, description of oil reservoirs, or gas migration around a nuclear waste repository in the subsurface. The numerical simulation of such flows is a challenging task. One well-known reason, which is the main topic of this paper, is that the capillary pressure and the relative permeability functions may be discontinuous across the interface between different regions of the domain.

We consider in this paper a simplified two-phase flow model (one equation, no advection) introduced in [21] to study the phenomenon of oil or gas trapping in a porous medium with several rock types. The main theoretical and numerical difficulties of this problem are the *nonlinearity* and *degeneracy* of the parabolic equation for the saturation of one of the phases, together with *nonlinear* and *discontinuous transmission*

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*conditions* at the interface between the rocks. Existence of a weak solution has been proven in [21], using the convergence of a finite volume scheme (see also [14, 15] and [12] for the full two-phase flow model). Uniqueness of a weak solution has been proven in [14] for a particular choice of functions characterizing the porous medium and in [16, 15] for the full two-phase problem with advection terms in the one-dimensional case. An a priori convergence study of a finite volume discretization has been undertaken in [21]. Due to different hydrogeological properties of the different rocks, domain decomposition (DD) methods appear to be a natural way to solve efficiently two-phase flow problems, and are proposed in [45, 46], see also [27, 41, 42].

The first purpose of this paper is to propose a *domain decomposition method* that is *global-in-time*, with time-dependent, nonlinear, and discontinuous optimized Ventcell transmission conditions at the interface between rock types, for solving the two-phase flow model of [21]. This method is based on the optimized Schwarz waveform relaxation algorithm (OSWR), in which at each OSWR iteration, space-time nonlinear subdomain problems over the whole time interval are solved. The exchange between the subdomains is here ensured using the nonlinear Ventcell transmission operators. Crucially, this approach allows for *different time stepping* in different parts of the domain, adapted to the physical properties of each subdomain, and for *parallelization in time*, in contrast to the domain decomposition algorithms discussed above. We are not aware of any domain decomposition algorithm proposed and analyzed for simultaneously a) degenerate parabolic problems; b) nonlinear and discontinuous transmission conditions; c) Robin and Ventcell transmission conditions; d) global-in-time formulation. Some of these ingredients have appeared previously independently as in [10, 11, 12, 28, 29, 31] and the references therein. The use of higher-order (Ventcell) transmission operators allows physically more valuable information exchanged between the subdomains and hence typically leads to a better convergence behavior, see [10, 26, 29, 31, 32, 33, 36] and the references therein for linear problems, and [13, 28] for problems with nonlinear reaction terms. The Robin case, obtained by setting one of the Ventcell parameters to zero, is analyzed in [2], both for the convergence of the space-time DD method, as well as for the existence of a weak solution of the subdomain problem with Robin boundary conditions.

The second purpose of this paper is to derive *a posteriori error estimates* for the finite volume – backward Euler approximation of the proposed space-time DD algorithm. We build here on the (few) previous contributions on unsteady, nonlinear, and degenerate problems in [37, 17, 20]; we will in particular rely on [20, Theorem 5.2], where the degenerate nature of the problem is handled to obtain an energy-type upper bound on the error. Two additional specific difficulties that were to the best of our knowledge not treated previously are that the current problem features nonlinear and discontinuous transmission conditions and that our finite volume discretization leads to an approximate solution that is nonconforming in space.

Finally, the third purpose of this paper is to address the question of when to *stop* the domain decomposition *iterations*, as well as the iterations of the linearization solver used for the subdomain problems. In contrast to prevalent practice, where one iterates until some fixed tolerance has been reached, we want to stop when the DD/linearization error component is up to a user-specified fraction below the total error. This typically spares numerous iterations. In practice, this means that the a posteriori error estimates we develop have to hold true at *each iteration* of the OSWR algorithm and the linearization, and distinguish the different error components (space, time, linearization, and domain decomposition). For this part of our work, we take up the path initiated in [9, 7, 34, 23, 44] for general techniques taking into account inexact algebraic solvers, [38] for (multiscale) mortar techniques, [39, 40] for FETI and BDD domain decomposition algorithms combined with conforming finite element discretizations, and most closely [4, 5] for respectively steady and unsteady linear problems with similar space and time discretizations. To achieve our goals here, we use a) equilibrated  $\mathbf{H}(\text{div})$ -conforming flux reconstructions, piecewise constant in time, that are direct extension of [5, 22, 44] to our model; b) novel subdomain-wise  $H^1$ -conforming saturation reconstructions, continuous and piecewise affine in time, which are targeted to the present setting in that they satisfy the nonlinear and discontinuous interface conditions.

The outline of the paper is as follows: section 2 recalls the physical model and defines weak solutions as well as the relevant functions spaces. section 3 presents the space-time domain decomposition method with nonlinear and discontinuous Ventcell transmission conditions. In section 4, we present the discrete OSWR algorithm, by combining a finite volume scheme for the discretization in the individual subdomains and the backward Euler time stepping with the OSWR method. We then construct the needed ingredients for the a posteriori error estimates: section 5 defines the postprocessing as well as the  $H^1$ - and  $\mathbf{H}(\text{div})$ -conforming reconstructions. section 6 puts the pieces together by presenting a guaranteed and fully computable error estimate that bounds the error between the unknown exact solution and the approximate solution. In

section 7 we decompose this overall estimator into individual estimators characterizing the space, time, domain decomposition, and linearization error components. This is used in section 8 to propose stopping criteria for the OSWR algorithm and for the nonlinear iterations. The method is numerically validated on three examples in three space dimensions in section 9. Finally, section 10 draws some conclusions.

## 2 Presentation of the problem

Let  $\Omega$  be an open bounded domain of  $\mathbb{R}^d$ ,  $d = 2$  or  $3$ , which is assumed to be polygonal if  $d = 2$  and polyhedral if  $d = 3$ . We denote by  $\partial\Omega$  its boundary (supposed to be Lipschitz-continuous) and by  $\mathbf{n}$  the unit normal to  $\partial\Omega$ , outward to  $\Omega$ . Let a time interval  $(0, T)$  be given with  $T > 0$ . We consider a simplified model of a two-phase flow through a heterogeneous porous medium, in which the advection is neglected. Assuming that there are only two phases occupying the porous medium  $\Omega$ , say gas and water, and that each phase is composed of a single component, the mathematical form of this problem as it is presented in [21, 14] is as follows: given initial and boundary gas saturations  $u_0$  and  $g$ , as well as a source term  $f$ , find  $u : \Omega \times [0, T] \rightarrow [0, 1]$  such that

$$\partial_t u - \nabla \cdot (\lambda(u, \mathbf{x}) \nabla \pi(u, \mathbf{x})) = f, \quad \text{in } \Omega \times (0, T), \quad (2.1a)$$

$$u(\cdot, 0) = u_0, \quad \text{in } \Omega, \quad (2.1b)$$

$$u = g, \quad \text{on } \partial\Omega \times (0, T). \quad (2.1c)$$

Here  $u$  is the *gas saturation* (and therefore  $(1 - u)$  is the water saturation),  $\pi(u, \mathbf{x}) : [0, 1] \times \Omega \rightarrow \mathbb{R}$  is the *capillary pressure*, and  $\lambda(u, \mathbf{x}) : [0, 1] \times \Omega \rightarrow \mathbb{R}$  is the *global mobility* of the gas. For simplicity, we consider only Dirichlet boundary conditions on  $\partial\Omega$ . Other types of boundary conditions could be dealt with the same way as in [14, 21, 44]. The model problem given by (2.1a) is a nonlinear degenerate parabolic problem as the global mobility  $\lambda(u) \rightarrow 0$  for  $u \rightarrow 0$  and  $1$ , and, moreover,  $\pi'(u) \rightarrow 0$  for  $u \rightarrow 0$  (see [8, 18]).

### 2.1 Flow between two rock types

In this part, we particularize the model problem (2.1a) to a porous medium with different capillary pressure curves  $\pi_i$  in each subdomain, following [21]. We suppose that  $\Omega$  is composed of two disjoint subdomains  $\Omega_i$ ,  $i = 1, 2$ , which are both open polygonal subsets of  $\mathbb{R}^d$  with Lipschitz-continuous boundary. We denote by  $\Gamma$  the interface between  $\Omega_1$  and  $\Omega_2$ , i.e.,  $\Gamma = (\partial\Omega_1 \cap \partial\Omega_2)^\circ$ . Let  $\Gamma_i^D = \partial\Omega_i \cap \partial\Omega$ . Both data  $\lambda$  and  $\pi$ , which can in general depend on the physical characteristics of the rock, are henceforth supposed to be homogeneous in each subdomain  $\Omega_i$ ,  $i = 1, 2$ , i.e.,  $\lambda_i(\cdot) := \lambda|_{\Omega_i}(\cdot) = \lambda(\cdot, \mathbf{x}), \forall \mathbf{x} \in \Omega_i$ , and similarly for  $\pi_i$ . The equations (2.1a) in *each subdomain*  $\Omega_i$  then read as

$$\partial_t u_i - \nabla \cdot (\lambda_i(u_i) \nabla \pi_i(u_i)) = f_i, \quad \text{in } \Omega_i \times (0, T), \quad (2.2a)$$

$$u_i(\cdot, 0) = u_0, \quad \text{in } \Omega_i, \quad (2.2b)$$

$$u_i = g_i, \quad \text{on } \Gamma_i^D \times (0, T). \quad (2.2c)$$

We use the notation  $v_i = v|_{\Omega_i}$  for an arbitrary function  $v$ .

Before transcribing the transmission conditions on the interface  $\Gamma$ , we make precise the assumptions on the data (further generalizations are possible, bringing more technicalities):

- Assumption 2.1** (Data). *1. For  $i \in \{1, 2\}$ ,  $\pi_i \in C^1([0, 1], \mathbb{R})$  can be extended in a continuous way to a function (still denoted by  $\pi_i$ ) such that  $\pi_i(u) = \pi_i(0)$  for all  $u \leq 0$  and  $\pi_i(u) = \pi_i(1)$  for all  $u \geq 1$ . Moreover,  $\pi_i|_{[0, 1]}$  is a strictly increasing function.*
- 2. For  $i \in \{1, 2\}$ ,  $\lambda_i \in C^0([0, 1], \mathbb{R}^+)$  is bounded and can be extended in a continuous way to a function (still denoted by  $\lambda_i$ ) such that  $\lambda_i(u) = \lambda_i(0)$  for all  $u \leq 0$  and  $\lambda_i(u) = \lambda_i(1)$  for all  $u \geq 1$ . We denote by  $C_\lambda$  an upper bound of  $\lambda_i(u)$ ,  $u \in \mathbb{R}$ .*
- 3. The initial condition is such that  $u_0 \in L^\infty(\Omega)$  with  $0 \leq u_0 \leq 1$  a.e. in  $\Omega$ .*

4. The boundary conditions  $0 \leq g_i \leq 1$  are traces of some functions from  $L^2(0, T; H^1(\Omega_i))$ . For simplicity, we suppose them at most piecewise second-order polynomials with respect to the boundary faces of the spatial mesh introduced in section 4.1.1 below, continuous on  $\Gamma_i^D$ , and constant in time. Moreover, they need to match in the sense that  $\pi_1(g_1(\mathbf{x})) = \pi_2(g_2(\mathbf{x}))$  for all  $\mathbf{x} \in \Gamma \cap \Gamma_1^D$  and all  $\mathbf{x} \in \Gamma \cap \Gamma_2^D$ .
5. The source term is such that  $f \in L^2(0, T; L^2(\Omega))$ . For simplicity we further assume that  $f$  is piecewise constant in time with respect to the temporal mesh introduced in section 4.1.2 below.

We give now the *transmission conditions* needed to connect the subdomain problems (2.2), for  $i = 1, 2$ . We consider two cases. The first case is when

$$\pi_1(0) = \pi_2(0) \quad \text{and} \quad \pi_1(1) = \pi_2(1), \quad (2.3)$$

the same way as in [14]. If the functions  $\pi_i$  satisfy the above condition, the capillarity curves are said to be matching and the resulting transmission conditions on the interface are given by

$$\pi_1(u_1) = \pi_2(u_2), \quad \text{on } \Gamma \times (0, T), \quad (2.4a)$$

$$\lambda_1(u_1) \nabla \pi_1(u_1) \cdot \mathbf{n}_1 = -\lambda_2(u_2) \nabla \pi_2(u_2) \cdot \mathbf{n}_2, \quad \text{on } \Gamma \times (0, T). \quad (2.4b)$$

These conditions yield a discontinuous saturation across the interface, i.e., we find that in general  $u_1 \neq u_2$  on  $\Gamma$ .

In the second case, i.e., in the case when

$$\pi_1(0) \neq \pi_2(0) \quad \text{or} \quad \pi_1(1) \neq \pi_2(1), \quad (2.5)$$

the capillarity pressure curves are said to be non-matching. Consequently, not only the saturation is discontinuous at the medium interface, but also the capillary pressure field. The condition (2.5), studied in [21], has direct consequences on the behavior of the capillary pressures on both sides of the interface  $\Gamma$ . Indeed, suppose that  $\pi_1(0) \leq \pi_2(0) < \pi_1(1) \leq \pi_2(1)$ , that  $u_1^*$  is the unique real in  $[0, 1]$  satisfying  $\pi_1(u_1^*) = \pi_2(0)$ , and that  $u_2^*$  is the unique real in  $[0, 1]$  satisfying  $\pi_2(u_2^*) = \pi_1(1)$ . Then, if  $u_1 \geq u_1^*$  and  $u_2 \leq u_2^*$ , we can still on the interface  $\Gamma$  prescribe the connection of the capillary pressures  $\pi_1(u_1) = \pi_2(u_2)$  as in (2.4a). If  $0 \leq u_1 \leq u_1^*$ , the model imposes  $u_2 = 0$ , and the gas phase is entrapped in the rock  $\Omega_1$ , and the water flows across  $\Gamma$ . In the same way, if  $u_2^* \leq u_2 \leq 1$ , the model prescribes  $u_1 = 1$ , and the water phase is captured in  $\Omega_2$  as a discontinuous phase, and the gas flows across  $\Gamma$  (see Fig. 1 left). Following [18, 21], these conditions on the gas-water saturations on the interface  $\Gamma$  are simply given by

$$\bar{\pi}_1(u_1) = \bar{\pi}_2(u_2), \quad \text{on } \Gamma \times (0, T), \quad (2.6a)$$

$$\lambda_1(u_1) \nabla \pi_1(u_1) \cdot \mathbf{n}_1 = -\lambda_2(u_2) \nabla \pi_2(u_2) \cdot \mathbf{n}_2, \quad \text{on } \Gamma \times (0, T), \quad (2.6b)$$

where  $\bar{\pi}_i$ , for  $i = 1, 2$ , are truncated capillary pressure functions given on  $[0, 1]$  respectively by  $\bar{\pi}_1 : u \mapsto \max(\pi_1(u), \pi_2(0))$  and  $\bar{\pi}_2 : u \mapsto \min(\pi_2(u), \pi_1(1))$  (see Fig. 1 right). In [21], it has been established that the model problem (2.2) together with the transmission conditions (2.6) has the necessary mathematical properties to explain the phenomena of gas trapping (see also [6, 16]).

## 2.2 Transformation of the equations and weak formulation

Still following [21], we present here the mathematical quantities and function spaces used to characterize the weak solution to the multidomain problem (2.2) with the conditions (2.6). That of the problem (2.2) with the conditions (2.4) can be deduced straightforwardly from this later, see [14]. As  $\Omega_i$  is a homogeneous rock type, so that  $\pi_i$  and  $\lambda_i$  do not depend on  $\mathbf{x}$ , one can define the Kirchhoff transform

$$\varphi_i : \begin{cases} [0, 1] & \longrightarrow \mathbb{R}^+ \\ s & \longmapsto \int_0^s \lambda_i(a) \pi_i'(a) da. \end{cases} \quad (2.7)$$

The function  $\varphi_i$  is Lipschitz-continuous and increasing on  $[0, 1]$ , and we denote by  $L_{\varphi,i}$  its Lipschitz constant, i.e.,  $L_{\varphi,i} := \max_{s \in [0,1]} \lambda_i(s) \pi_i'(s)$ , so that

$$|\varphi_i(a) - \varphi_i(b)| \leq L_{\varphi,i} |a - b|, \quad \forall (a, b) \in [0, 1]^2,$$

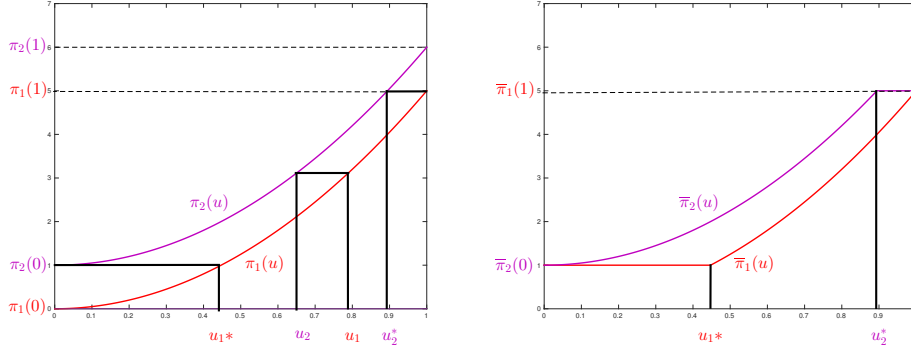


Figure 1: Capillary pressure curves (left) and truncated capillary pressures curves (right)

and we let  $L_\varphi := \max(L_{\varphi,1}, L_{\varphi,2})$ . We extend the function  $\varphi_i$  from  $[0, 1]$  to  $\mathbb{R}$  so that  $\varphi_i(u) = \varphi_i(0)$  for all  $u \leq 0$  and  $\varphi_i(u) = \varphi_i(1)$  for all  $u \geq 1$ .

We now introduce the strictly increasing function  $\phi$  by

$$\phi : \begin{cases} [\pi_2(0), \pi_1(1)] & \longrightarrow \mathbb{R}^+ \\ s & \longmapsto \int_{\pi_2(0)}^s \min_{j \in \{1,2\}} (\lambda_j \circ \pi_j^{-1}(a)) da, \end{cases}$$

and let  $\Pi_i := \phi \circ \bar{\pi}_i$ , for  $i \in \{1, 2\}$ . The functions  $\Pi_i|_{[0,1]}$ , introduced first in [21, Lemma 1.2] and used in [14, 16, 2], are differentiable and increasing. We let  $\Pi_i(u) = \Pi_i(0)$  for all  $u \leq 0$  and  $\Pi_i(u) = \Pi_i(1)$  for all  $u \geq 1$  and define the function  $\Pi$  by

$$\Pi(u, \mathbf{x}) = \Pi_i(u), \quad \text{for } \mathbf{x} \in \Omega_i.$$

As  $\Pi_i$  are more regular than  $\bar{\pi}_i$ , this allows to connect  $\Pi_1$  and  $\Pi_2$  instead of  $\bar{\pi}_1$  and  $\bar{\pi}_2$ , that is, for all  $(u_1, u_2) \in \mathbb{R}^2$ , we have the crucial *equivalence property*

$$\bar{\pi}_1(u_1) = \bar{\pi}_2(u_2) \Leftrightarrow \Pi_1(u_1) = \Pi_2(u_2).$$

Finally, under Assumption 2.1, the function  $\Pi_i \circ \varphi_i^{-1}$  is Lipschitz-continuous with a Lipschitz constant lower than 1 (see [21, Lemma 1.2]), i.e.

$$|\Pi_i(a) - \Pi_i(b)| \leq |\varphi_i(a) - \varphi_i(b)|, \quad \forall (a, b) \in [0, 1]^2. \quad (2.8)$$

This inequality will be used in Remark 6.3 below.

We now apply the Kirchhoff transformation (2.7) separately in each subdomain, giving an equivalent formulation suitable for *mathematical analysis*: find  $u_i$  such that

$$\partial_t u_i - \Delta \varphi_i(u_i) = f_i, \quad \text{in } \Omega_i \times (0, T), \quad (2.9a)$$

$$u_i(\cdot, 0) = u_0, \quad \text{in } \Omega_i, \quad (2.9b)$$

$$\varphi_i(u_i) = \varphi_i(g_i), \quad \text{on } \Gamma_i^D \times (0, T), \quad (2.9c)$$

together with the conditions at the interface relying on the smoother functions  $\Pi_i$

$$\Pi_1(u_1) = \Pi_2(u_2), \quad \text{on } \Gamma \times (0, T), \quad (2.10a)$$

$$\nabla \varphi_1(u_1) \cdot \mathbf{n}_1 = -\nabla \varphi_2(u_2) \cdot \mathbf{n}_2, \quad \text{on } \Gamma \times (0, T). \quad (2.10b)$$

In general, the multidomain problem (2.9)–(2.10) does not have any strong solution, but the introduction of the Kirchhoff transforms  $\varphi_i$  and of the smoother functions  $\Pi_i$  will, following [21], allow for a definition of a weak solution. To this aim, we define

$$\begin{aligned} X_{\varphi_i(g_i)} &:= L^2(0, T; H^1_{\varphi_i(g_i)}(\Omega_i)), \\ X_{\Pi(g, \cdot)} &:= L^2(0, T; H^1_{\Pi(g, \cdot)}(\Omega)), \quad X := L^2(0, T; H^1_0(\Omega)), \end{aligned}$$

where  $H^1_{\varphi_i(g_i)}(\Omega_i) := \{v \in H^1(\Omega_i), v = \varphi_i(g_i) \text{ on } \Gamma_i^D\}$  and similarly  $H^1_{\Pi(g,\cdot)}(\Omega) := \{v \in H^1(\Omega), v = \Pi(g, \cdot) \text{ on } \partial\Omega\}$ .

We equip the space  $X$  with the norm

$$\|\psi\|_X := \left\{ \int_0^T \|\nabla\psi(\cdot, t)\|_{L^2(\Omega)}^2 dt \right\}^{\frac{1}{2}}.$$

The dual space of  $X$  is

$$X' := L^2(0, T; H^{-1}(\Omega)). \quad (2.11)$$

We will use the notation  $\langle \cdot, \cdot \rangle_{H^{-1}(\Omega), H^1_0(\Omega)}$  to denote the duality pairing between  $H^{-1}(\Omega)$  and  $H^1_0(\Omega)$ . We will also need the space

$$Z := H^1(0, T; H^{-1}(\Omega)).$$

Using the above developments, a *weak solution* to problem (2.9)–(2.10) is defined as:

**Definition 2.2** (Weak solution). *We say that a function  $u$  is a weak solution to problem (2.9)–(2.10) if it satisfies:*

1.  $u \in Z$ ;
2.  $u(\cdot, 0) = u_0$ ;
3.  $\varphi_i(u_i) \in X_{\varphi_i(g_i)}$ , where  $u_i := u|_{\Omega_i}$ ,  $i = 1, 2$ ;
4.  $\Pi(u, \cdot) \in X_{\Pi(g,\cdot)}$ ;
5. For all  $\psi \in X$ , the following integral equality holds:

$$\int_0^T \left\{ \langle \partial_t u, \psi \rangle_{H^{-1}(\Omega), H^1_0(\Omega)} + \sum_{i=1}^2 (\nabla\varphi_i(u_i), \nabla\psi)_{\Omega_i} - (f, \psi) \right\} dt = 0.$$

In this paper, we assume that a weak solution given by Definition 2.2 exists. One can then easily show that  $\Pi$  has sufficient regularity to impose the condition (2.10a). Indeed, since  $\Pi_i \circ \varphi_i^{-1}$  is a Lipschitz-continuous function, the third point of Definition 2.2 ensures that  $\Pi_i(u_i)$  belongs to  $L^2(0, T; H^1(\Omega_i))$ ,  $i = 1, 2$ . Thus, the point 4 of Definition 2.2 implies the continuity condition (2.10a). Finally, when supposing additionally that the weak solution  $u$  is sufficiently regular so that  $\partial_t u \in L^2(0, T; L^2(\Omega))$ , condition (2.10b) is satisfied weakly using point 5 of Definition 2.2.

**Remark 2.3** (Existence and uniqueness of a weak solution). *In [21], the existence of a weak solution to problem (2.9)–(2.10) (with homogeneous Neumann boundary conditions) was proved using integration by parts for the time term which requires a stronger test function space. Using the imposed conditions, one also finds  $u \in L^\infty(0, T; L^\infty(\Omega))$ , with  $0 \leq u \leq 1$  a.e. in  $\Omega \times (0, T)$ . In fact, in [21] (see also [14]), the derived weak solution is given as the limit of a finite volume approximation of the solution refining the space and time discretization, and requires a stronger test function space for the application of the Kolmogorov compactness criterion in  $L^\infty$ . For the uniqueness, a first result was obtained in [14] for the case of matching capillary pressures curves. For the more general case, the uniqueness is demonstrated only for the one-dimensional case in [15].*

### 3 Space-time domain decomposition with Ventcell transmission conditions

This section proposes our global-in-time domain decomposition method for the degenerate parabolic problem (2.9) with the nonlinear and discontinuous interface conditions (2.10). We in particular design appropriate Robin and Ventcell transmission conditions.

An equivalent formulation to the model problem (2.9)–(2.10) can be obtained by solving, for  $i = 1, 2$ , equations (2.9) together with optimized Ventcell transmission conditions on  $\Gamma \times (0, T)$

$$\nabla \varphi_1(u_1) \cdot \mathbf{n}_1 + \mathcal{L}_1(\Pi_1(u_1)) = -\nabla \varphi_2(u_2) \cdot \mathbf{n}_2 + \mathcal{L}_1(\Pi_2(u_2)), \quad (3.1a)$$

$$\nabla \varphi_2(u_2) \cdot \mathbf{n}_2 + \mathcal{L}_2(\Pi_2(u_2)) = -\nabla \varphi_1(u_1) \cdot \mathbf{n}_1 + \mathcal{L}_2(\Pi_1(u_1)), \quad (3.1b)$$

where  $\mathcal{L}_i$ ,  $i = 1, 2$ , is a *Ventcell* (or second-order) *boundary operator* defined by

$$\mathcal{L}_i(v) := \alpha_{i,j} v + \gamma_{i,j} (\partial_t v - \Delta_\Gamma v), \quad j = (3 - i), \quad (3.2)$$

for a sufficiently regular function  $v$  defined on  $\Gamma \times (0, T)$ , where  $\Delta_\Gamma$  represents the Laplace operator on  $\Gamma$  (the Laplace–Beltrami operator). The *Robin transmission conditions* are simply obtained by taking in (3.2) the parameters  $\gamma_{i,j} = 0$ . One can easily show that the operators  $\mathcal{L}_i$  involve not only the continuity of the function  $\Pi$  as for the Robin case, but also the continuity of the time derivative and of the second-order derivatives of  $\Pi$  along the interface. As a result, this formulation can be seen as a coupling problem between a  $d$ -dimensional PDE in the rock  $\Omega_i$  and a  $(d - 1)$ -dimensional PDE on the interface  $\Gamma$  between the rock types, which greatly enhances the information exchange between the solutions in the subdomains, see [33, 26, 13, 29] for some model cases.

The Ventcell–OSWR algorithm is defined as follows: the solution  $u$  in the whole domain  $\Omega$  given by  $u_i = u|_{\Omega_i}$  is approximated by a sequence of solutions  $u_i^k$ ,  $k \geq 1$ , defined recursively by

$$\partial_t u_i^k - \Delta \varphi_i(u_i^k) = f_i, \quad \text{in } \Omega_i \times (0, T), \quad (3.3a)$$

$$u_i^k(\cdot, 0) = u_0, \quad \text{in } \Omega_i, \quad (3.3b)$$

$$\varphi_i(u_i^k) = \varphi_i(g_i), \quad \text{on } \Gamma_i^D \times (0, T), \quad (3.3c)$$

$$\nabla \varphi_i(u_i^k) \cdot \mathbf{n}_i + \mathcal{L}_i(\Pi_i(u_i^k)) = \Psi_i^{k-1}, \quad \text{on } \Gamma \times (0, T), \quad (3.3d)$$

with

$$\Psi_i^{k-1} := -\nabla \varphi_j(u_j^{k-1}) \cdot \mathbf{n}_j + \mathcal{L}_i(\Pi_j(u_j^{k-1})), \quad j = (3 - i), \quad k \geq 2, \quad (3.4)$$

and  $\Psi_i^0$  is an initial Ventcell guess on  $\Gamma \times (0, T)$ .

**Remark 3.1** (Interface operators). *The multi-domain problem (2.9) together with the transmission conditions (3.1) can be formulated through the use of interface operators as a problem posed on the space-time interface, see [2], where Robin-to-Robin conditions are analyzed, and also [31, 32]. This interface problem can be solved iteratively by using fixed point iterations (which corresponds to the OSWR algorithm above) or via a Newton–Krylov method.*

**Remark 3.2** (Domain decomposition algorithm in physical variables). *The algorithm (3.3)–(3.4) is written in the variables  $\varphi_i(u_i^k)$  and  $\Pi_i(u_i^k)$  stemming from the rewriting (2.9)–(2.10) and the corresponding weak formulation of Definition 2.2. One could also formulate a Ventcell–OSWR domain decomposition algorithm directly in the physical variables, using the original formulation (2.2) and the corresponding transmission conditions (2.6):*

$$\partial_t u_i^k - \nabla \cdot (\lambda_i(u_i^k) \nabla \pi_i(u_i^k)) = f_i, \quad \text{in } \Omega_i \times (0, T), \quad (3.5a)$$

$$u_i^k(\cdot, 0) = u_0, \quad \text{in } \Omega_i, \quad (3.5b)$$

$$u_i^k = g_i, \quad \text{on } \Gamma_i^D \times (0, T), \quad (3.5c)$$

$$\lambda_i(u_i^k) \nabla \pi_i(u_i^k) \cdot \mathbf{n}_i + \bar{\mathcal{L}}_i(u_i^k) = \Psi_i^{k-1}, \quad \text{on } \Gamma \times (0, T), \quad (3.5d)$$

with

$$\begin{aligned} \bar{\mathcal{L}}_i(u_i^k) &:= \alpha_{i,j} \bar{\pi}_i(u_i^k) + \gamma_{i,j} (\partial_t u_i^k - \nabla_{\Gamma} \cdot (\lambda_i(u_i^k) \nabla \pi_i(u_i^k))), \quad j = (3 - i), \\ \Psi_i^{k-1} &:= -\lambda_j(u_j^{k-1}) \nabla \pi_j(u_j^{k-1}) \cdot \mathbf{n}_j + \bar{\mathcal{L}}_i(u_i^k), \quad j = (3 - i), \quad k \geq 2, \end{aligned} \quad (3.6)$$

and  $\Psi_i^0$  is an initial Ventcell guess on  $\Gamma \times (0, T)$ .

Though algorithms (3.3)–(3.4) and (3.5)–(3.6) may differ, an a posteriori error analysis of both algorithms can be done simultaneously as in [17], see the “mathematical” scheme of Definition 4.1 and the “engineering” scheme of Definition 4.4 therein. Indeed, [17, Theorem 3.3] applies to both schemes. We avoid this here for the sake of conciseness.



## 4 Cell-centered finite volume scheme

We present here a finite volume discretization of the OSWR algorithm (3.3)–(3.4); we also develop linearization of the subdomain problems by the Newton method, used later in the a posteriori analysis.

### 4.1 Space-time discretization, notations, and function spaces

We introduce here partitions of  $\Omega$  and  $\Gamma$ , time discretization, and discrete function spaces.

#### 4.1.1 Partitions of $\Omega$ and $\Gamma$

Let  $\mathcal{T}_{h,i}$  be a partition of the subdomain  $\Omega_i$  into elements  $K$ , such that  $\overline{\Omega}_i = \cup_{K \in \mathcal{T}_{h,i}} K$ ; here we suppose that they are either simplices or rectangular parallelepipeds but general elements can be treated via submeshes, see [19] and the references therein. Moreover, we assume that the partition is conforming in the sense that if  $K, L \in \mathcal{T}_{h,i}$ ,  $K \neq L$ , then  $K \cap L$  is either an empty set, a common face, edge, or vertex of  $K$  and  $L$ .

We then set  $\mathcal{T}_h = \cup_{i=1}^2 \mathcal{T}_{h,i}$  and denote by  $h$  the maximal element diameter in  $\mathcal{T}_h$ . The meshes are supposed to be matching on the interface  $\Gamma$ . For all  $K \in \mathcal{T}_h$ ,  $h_K$  denotes the diameter of the mesh element  $K$  and  $|K|$  its volume. The interior mesh faces in  $\mathcal{T}_{h,i}$  are collected into the set  $\mathcal{E}_{h,i}^{\text{int}}$ ; hence  $\mathcal{E}_{h,i}^{\text{int}}$  contains neither the subdomain interfaces nor the outer boundary of  $\Omega$ . The faces of  $\mathcal{T}_{h,i}$  lying on  $\Gamma_i^{\text{D}}$  are collected in the set  $\mathcal{E}_{h,i}^{\text{D}}$ . We denote by  $\mathcal{E}_{h,i}$  all the faces of  $\mathcal{T}_{h,i}$  and we set  $\mathcal{E}_h = \cup_{i=1}^2 \mathcal{E}_{h,i}$ . The notation  $\mathcal{E}_K$  stands for all the faces of an element  $K \in \mathcal{T}_h$ . Let  $\mathcal{E}_h^\Gamma$  be a partition of  $\Gamma$  given by the faces of  $\mathcal{T}_h$  on  $\Gamma$ . We use also  $\mathcal{F}_{h,i}^{\text{int}}$  to denote the interior sides (these are the points (if  $d = 2$ ) or edges (if  $d = 3$ )) of  $\mathcal{E}_{h,i}^{\text{int}}$ . We denote by  $\mathcal{F}_{h,i}^{\text{D}}$  the sides of  $\mathcal{E}_{h,i}^{\text{D}}$  on  $\Gamma_i^{\text{D}}$ . The sides of a face  $\sigma \in \mathcal{E}_h$  are collected in the set  $\mathcal{F}_\sigma$ . The volume of a face  $\sigma$  is denoted by  $|\sigma|$  and that of a side  $e$  by  $|e|$ . Finally, we use the notation  $\mathbf{x}_K$  to denote the ‘‘center’’ of the cell  $K \in \mathcal{T}_h$ . If  $\sigma = K|L \in \mathcal{E}_h$  separates the cells  $K$  and  $L$ ,  $d_{K,L}$  denotes the Euclidean distance between  $\mathbf{x}_K$  and  $\mathbf{x}_L$ , and  $d_{K,\sigma}$  for  $\sigma \in \mathcal{E}_K$  denotes the distance from  $\mathbf{x}_K$  to  $\sigma$ . Similarly, we let  $\mathbf{x}_\sigma$  be the ‘‘center’’ of the face  $\sigma$  and  $\mathbf{x}_e$  the ‘‘center’’ of the edge  $e$  and denote respectively by  $d_{\sigma,\tilde{\sigma}}$  and  $d_{\sigma,e}$  the distance between  $\mathbf{x}_\sigma$  and  $\mathbf{x}_{\tilde{\sigma}}$  for  $e = \sigma|\tilde{\sigma} \in \mathcal{F}_{h,i}^{\text{int}}$  and the distance from  $\mathbf{x}_\sigma$  to  $e$  for  $e \in \mathcal{F}_\sigma$ .

We assume that the composite mesh  $\mathcal{T}_h$  satisfies the following orthogonality condition: for an interface  $\sigma = K|L$ , the line segment  $\mathbf{x}_K \mathbf{x}_L$  is orthogonal to this interface (see [24]). The same condition should be satisfied for a side  $e = \sigma|\tilde{\sigma} \in \mathcal{F}_{h,i}^{\text{int}}$  due to the discretization of the Ventcell operator (see Fig. 2).

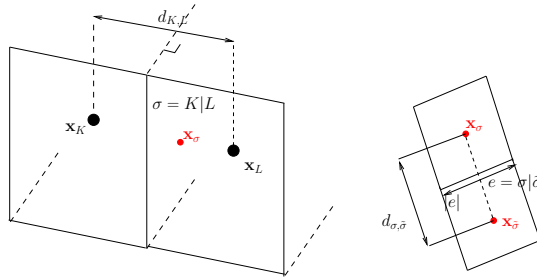


Figure 2: Notation for admissible meshes in three space dimensions

#### 4.1.2 Time discretization

For an integer  $N \geq 0$ , let  $(\tau^n)_{0 \leq n \leq N}$  denote a sequence of positive real numbers corresponding to the discrete time steps such that  $T = \sum_{n=1}^N \tau^n$ . Let  $t_0 = 0$ , and  $t^n = \sum_{j=1}^n \tau^j$ ,  $1 \leq n \leq N$ , be the discrete times. Let  $I^n = (t^{n-1}, t^n]$ ,  $1 \leq n \leq N$ . For simplicity, we consider only conforming time grids. The analysis remains valid if we use different time steps in the subdomains, as was done in [5] for a linear diffusion problem.

### 4.1.3 Notation and discrete function spaces

We denote by  $\mathbb{P}_l(S)$  the space of polynomials on a subdomain  $S \subset \Omega$  of total degree less than or equal to  $l$  and by

$$\mathbb{P}_l(\mathcal{T}_h) := \{p_h \in L^2(\Omega); p_h|_K \in \mathbb{P}_l(K), \forall K \in \mathcal{T}_h\},$$

the space of piecewise  $l$ -degree polynomials on  $\mathcal{T}_h$ . We use the notation  $\|\cdot\|_K$  for the norm in  $L^2(K)$ ,  $K \in \mathcal{T}_h$ . The corresponding inner product is  $(\cdot, \cdot)_K$ . We also denote by  $(\cdot, \cdot)_\sigma$  the inner product in  $L^2(\sigma)$  for  $\sigma \in \mathcal{E}_h$ . Let  $|S|$  be the Lebesgue measure of  $S$ , and  $|\sigma|$  the  $(d-1)$ -dimensional Lebesgue measure of  $\sigma \in \mathbb{R}^{d-1}$ . We define the broken Sobolev space  $H^1(\mathcal{T}_h)$  as the space of all functions  $v \in L^2(\Omega)$  such that  $v|_K \in H^1(K)$ , for all  $K \in \mathcal{T}_h$ . We will use the sign  $\nabla$  to denote the elementwise gradient, i.e., the gradient of a function restricted to a mesh element  $K \in \mathcal{T}_h$ . We define  $P_\tau^1(H^1(\mathcal{T}_h))$  and  $P_\tau^1(H_0^1(\Omega))$  as the space of continuous and piecewise affine in-time functions  $v_{h\tau}$  with values in  $H^1(\mathcal{T}_h)$  and in  $H_0^1(\Omega)$ , respectively. In both these situations, for every time step  $1 \leq n \leq N$ , we will use the abridged notation  $v_h^n := v_{h\tau}(\cdot, t^n)$ . By Assumption 2.1, the source function  $f$  is piecewise constant in time, i.e., constant on each time interval  $I^n$ ,  $1 \leq n \leq N$ . Its value on  $I^n$  is denoted by  $f^n := f|_{I^n}$ .

The domain decomposition method we consider is global in time. Thus, at the space-time interface  $\Gamma \times (0, T)$ , data should be transferred from one space-time subdomain to the neighboring subdomain. Then, we denote by  $P_\tau^0(L^2(\Gamma))$  the space of functions piecewise constant in time and with values in  $L^2(\Gamma)$ . Let  $\mathbf{H}(\text{div}, \Omega)$  be the space of vector-valued functions from  $[L^2(\Omega)]^d$  that admit a weak divergence in  $L^2(\Omega)$ . Recall that all functions in  $\mathbf{H}(\text{div}, \Omega)$  have a continuous normal trace across the interface  $\Gamma$ . As above,  $P_\tau^0(\mathbf{H}(\text{div}, \Omega))$  is the space of functions piecewise constant in time with values in  $\mathbf{H}(\text{div}, \Omega)$ . We use  $\mathbf{RTN}_0(\Omega)$  to denote the lowest-order Raviart–Thomas–Nédélec finite-dimensional subspace of  $\mathbf{H}(\text{div}, \Omega)$ ; any  $\mathbf{v}_h \in \mathbf{RTN}_0(\Omega)$  takes on each element  $K \in \mathcal{T}_h$  the form  $[\mathbb{P}_0(K)]^d + \mathbb{P}_0(K)\mathbf{x}$  for the example of simplices.

Finally, given a function  $v$  that is double-valued on the interface  $\Gamma$ , the jump and the average of  $v$  on a face  $\sigma \in \mathcal{E}_h^\Gamma$ ,  $\sigma = K|L$ ,  $K \in \mathcal{T}_{h,1}$ ,  $L \in \mathcal{T}_{h,2}$ , are defined as

$$[[v]] = (v_K)|_\sigma - (v_L)|_\sigma, \quad \{\{v\}\} = \frac{(v_K)|_\sigma + (v_L)|_\sigma}{2}.$$

Here  $v_K = v|_K$  is the restriction of  $v$  to the element  $K \in \mathcal{T}_h$ .

## 4.2 A space-time fully discrete scheme based on finite volumes in space and the backward Euler scheme in time

For the iteration  $k \geq 1$  of the OSWR algorithm (3.3)–(3.4), subdomain  $\Omega_i$ ,  $i = 1, 2$ , and the time steps  $0 \leq n \leq N$ , let the *discrete saturation*  $u_{h,i}^{k,n} \in \mathbb{P}_0(\mathcal{T}_{h,i}) \times \mathbb{P}_0(\mathcal{E}_h^\Gamma)$  be identified with the vector of unknowns

$$u_{h,i}^{k,n} := \left( (u_K^{k,n})_{K \in \mathcal{T}_{h,i}}, (u_{K,\sigma}^{k,n})_{\sigma \in \mathcal{E}_K \cap \mathcal{E}_h^\Gamma, K \in \mathcal{T}_{h,i}} \right).$$

Note that there are in total two interface unknowns  $u_{K,\sigma}^{k,n}$  for each face  $\sigma$  of  $\mathcal{E}_h^\Gamma$ , in addition to the usual one unknown  $u_K^{k,n}$  per mesh element.

We then define the discrete flux  $F_{K,\sigma}$  over a face  $\sigma \in \mathcal{E}_h \cap \mathcal{E}_K$ ,  $K \in \mathcal{T}_{h,i}$ , by

$$F_{K,\sigma}(u_{h,i}^{k,n}) := \begin{cases} \frac{\varphi_i(u_K^{k,n}) - \varphi_i(u_L^{k,n})}{d_{K,L}}, & \text{if } \sigma = K|L \in \mathcal{E}_{h,i}^{\text{int}}, \\ \frac{\varphi_i(u_K^{k,n}) - \varphi_i(g_i(\mathbf{x}_\sigma))}{d_{K,\sigma}}, & \text{if } \sigma \in \mathcal{E}_K \cap \mathcal{E}_{h,i}^{\text{D}}, \\ \frac{\varphi_i(u_K^{k,n}) - \varphi_i(u_{K,\sigma}^{k,n})}{d_{K,\sigma}}, & \text{if } \sigma \in \mathcal{E}_K \cap \mathcal{E}_h^\Gamma, \end{cases} \quad (4.1a)$$

and the discrete  $(d-1)$ -dimensional flux  $\bar{F}_{\sigma,e}$  over a side  $e \in \mathcal{F}_\sigma$ ,  $\sigma \in \mathcal{E}_K \cap \mathcal{E}_h^\Gamma$ , by

$$\bar{F}_{\sigma,e}(u_{h,i}^{k,n}) := \begin{cases} \frac{\Pi_i(u_{K,\sigma}^{k,n}) - \Pi_i(u_{K,\bar{\sigma}}^{k,n})}{d_{\sigma,\bar{\sigma}}}, & \text{if } e = \sigma|\bar{\sigma} \in \mathcal{F}_\sigma \cap \mathcal{F}_{h,i}^{\text{int}}, \\ \frac{\Pi_i(u_{K,\sigma}^{k,n}) - \Pi_i(g_i(\mathbf{x}_e))}{d_{\sigma,e}}, & \text{if } e \in \mathcal{F}_\sigma \cap \mathcal{F}_{h,i}^{\text{D}}. \end{cases} \quad (4.1b)$$

Using (4.1), the approximation of the solution  $u^k$  in the OSWR algorithm (3.3)–(3.4) is: at each iteration  $k \geq 1$ , the initial condition is given by

$$u_K^{k,0} = \frac{1}{|K|}(u_0, 1)_K, \quad \forall K \in \mathcal{T}_h, \quad (4.2a)$$

and for  $n = 1, \dots, N$ , the discrete saturation  $u_{h,i}^{k,n} \in \mathbb{P}_0(\mathcal{T}_{h,i}) \times \mathbb{P}_0(\mathcal{E}_h^\Gamma)$ ,  $i = 1, 2$ , is given by the following *finite volume scheme*:

$$\frac{u_K^{k,n} - u_K^{k,n-1}}{\tau^n} |K| + \sum_{\sigma \in \mathcal{E}_K} |\sigma| F_{K,\sigma}(u_{h,i}^{k,n}) = (f_i^n, 1)_K, \quad \forall K \in \mathcal{T}_{h,i}, \quad (4.2b)$$

$$-F_{K,\sigma}(u_{h,i}^{k,n}) + \gamma_{i,j} \frac{\Pi_i(u_{K,\sigma}^{k,n}) - \Pi_i(u_{K,\sigma}^{k,n-1})}{\tau^n} |\sigma| + \left( \Lambda_{K,\Gamma}(u_{h,i}^{k,n}) \right)_\sigma = \Psi_{L,\sigma}^{k-1,n}, \quad \forall \sigma = K|L \in \mathcal{E}_h^\Gamma, \quad (4.2c)$$

where, for  $K \in \mathcal{T}_{h,i}$ ,

$$\left( \Lambda_{K,\Gamma}(u_{h,i}^{k,n}) \right)_\sigma := \alpha_{i,j} |\sigma| \Pi_i(u_{K,\sigma}^{k,n}) + \gamma_{i,j} \sum_{e \in \mathcal{F}_\sigma} |e| \bar{F}_{\sigma,e}(u_{h,i}^{k,n}), \quad \sigma \in \mathcal{E}_K \cap \mathcal{E}_h^\Gamma \quad (4.2d)$$

and, for  $L \in \mathcal{T}_{h,j}$ ,  $j = 3 - i$ , and  $\sigma = K|L \in \mathcal{E}_h^\Gamma$ , the Ventcell information from  $\Omega_j$  is

$$\Psi_{L,\sigma}^{k-1,n} := F_{L,\sigma}(u_{h,j}^{k-1,n}) + \gamma_{i,j} \frac{\Pi_j(u_{L,\sigma}^{k-1,n}) - \Pi_j(u_{L,\sigma}^{k-1,n-1})}{\tau^n} |\sigma| + \left( \Lambda_{L,\Gamma}(u_{h,j}^{k-1,n}) \right)_\sigma. \quad (4.3)$$

### 4.3 Newton linearization

At *Newton linearization* step  $m \geq 1$  the following problem is obtained: find  $u_{h,i}^{k,n,m} := \left( (u_{K,\sigma}^{k,n,m})_{K \in \mathcal{T}_{h,i}}, (u_{K,\sigma}^{k,n,m})_{\sigma \in \mathcal{E}_K \cap \mathcal{E}_h^\Gamma, K \in \mathcal{T}_{h,i}} \right) \in \mathbb{P}_0(\mathcal{T}_{h,i}) \times \mathbb{P}_0(\mathcal{E}_h^\Gamma)$ , such that

$$\frac{u_K^{k,n,m} - u_K^{k,n-1}}{\tau^n} |K| + \sum_{\sigma \in \mathcal{E}_K} |\sigma| F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m}) = (f_i^n, 1)_K, \quad \forall K \in \mathcal{T}_{h,i}, \quad (4.4a)$$

$$-F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m}) + \gamma_{i,j} \frac{\Pi_i^{m-1}(u_{K,\sigma}^{k,n,m}) - \Pi_i^{m-1}(u_{K,\sigma}^{k,n-1})}{\tau^n} |\sigma| + \left( \Lambda_{K,\Gamma}^{m-1}(u_{h,i}^{k,n,m}) \right)_\sigma = \Psi_{L,\sigma}^{k-1,n}, \quad \forall \sigma = K|L \in \mathcal{E}_h^\Gamma, \quad (4.4b)$$

where  $F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m})$  are the linearized face fluxes given by

$$\begin{aligned} F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m}) &:= F_{K,\sigma}(u_{h,i}^{k,n,m-1}) + \sum_{M=K,L} \frac{\partial F_{K,\sigma}}{\partial u_M}(u_{h,i}^{k,n,m-1}) \cdot (u_M^{k,n,m} - u_M^{k,n,m-1}) \\ &+ \frac{\partial F_{K,\sigma}}{\partial u_{K,\sigma}}(u_{h,i}^{k,n,m-1}) \cdot (u_{K,\sigma}^{k,n,m} - u_{K,\sigma}^{k,n,m-1}), \end{aligned} \quad (4.5)$$

where the linearization of the function  $\Pi_i$  is

$$\Pi_i^{m-1}(u_{K,\sigma}^{k,n,m}) := \Pi_i(u_{K,\sigma}^{k,n,m-1}) + \frac{\partial \Pi_i}{\partial u_{K,\sigma}}(u_{K,\sigma}^{k,n,m-1}) \cdot (u_{K,\sigma}^{k,n,m} - u_{K,\sigma}^{k,n,m-1}),$$

and where finally

$$\begin{aligned} \left( \Lambda_{K,\Gamma}^{m-1}(u_{h,i}^{k,n,m}) \right)_\sigma &:= \left( \Lambda_{K,\Gamma}(u_{h,i}^{k,n,m-1}) \right)_\sigma + \alpha_{i,j} |\sigma| \frac{\partial \Pi_i}{\partial u_{K,\sigma}}(u_{K,\sigma}^{k,n,m-1}) \cdot (u_{K,\sigma}^{k,n,m} - u_{K,\sigma}^{k,n,m-1}) \\ &+ \gamma_{i,j} \sum_{e \in \mathcal{F}_\sigma} |e| \sum_{A=\sigma,\bar{\sigma}} \frac{\partial \bar{F}_{\sigma,e}}{\partial u_A}(u_{h,i}^{k,n,m-1}) \cdot (u_A^{k,n,m} - u_A^{k,n,m-1}). \end{aligned}$$

Equations (4.4a)–(4.4b) form a system of *linear algebraic equations* that is solved at each domain decomposition iteration  $k$ , time step  $n$ , and Newton iteration  $m$ , *independently in each of the subdomains*  $\Omega_i$ .

## 5 Postprocessing and $H^1$ - and $\mathbf{H}(\text{div})$ -conforming reconstructions

So far, we have described the OSWR domain decomposition algorithm and its finite volume discretization. In the next four sections, we address the important question of assessing the accuracy of the approximate solution, both as a function of the space and time discretization parameters, and as a function of the OSWR and Newton iterations. This is achieved by deriving detailed a posteriori error estimators for each of the possible error components.

At each OSWR iteration  $k \geq 1$ , time step  $0 \leq n \leq N$ , and linearization step  $m \geq 1$ , let  $u_{h\tau}^{k,m}$  be the piecewise constant in space and in time approximation of the saturation given by the values  $u_K^{k,n,m}$ ,  $K \in \mathcal{T}_h$ , defined in (4.4). In this section, we develop basic tools that will allow us to build the estimators. We extend for this purpose to the present setting the approach of [22, 38, 44, 20] and the references therein and proceed in three steps:

- (i) Define a *locally postprocessed saturation*  $\tilde{u}_{h\tau}^{k,m}$  that is elementwise more regular than  $u_{h\tau}^{k,m}$ . This is customary in finite volume methods, as an energy-norm-type a posteriori error estimate has no meaning for the piecewise constant  $u_{h\tau}^{k,m}$ . There, however, holds (recall that we use the notation  $\tilde{u}_{h\tau,i}^{k,m} = \tilde{u}_{h\tau}^{k,m}|_{\Omega_i}$ )

$$\varphi_i(\tilde{u}_{h\tau,i}^{k,m}) \notin X_{\varphi_i(g_i)}, \quad i = 1, 2, \quad \text{and} \quad \Pi_1(\tilde{u}_{h\tau,1}^{k,m}) \neq \Pi_2(\tilde{u}_{h\tau,2}^{k,m}) \quad \text{on } \Gamma, \quad (5.1)$$

since  $\tilde{u}_{h\tau}^{k,m}$  is discontinuous between mesh elements. Thus,  $\tilde{u}_{h\tau}^{k,m}$  is a *nonconforming approximation* of the weak solution of Definition 2.2 that has to in particular satisfy properties 3 and 4.

- (ii) Define a *saturation reconstruction*  $s_{h\tau}^{k,m}$  that is *conforming* in the sense of Definition 2.2, satisfying all

$$s_{h\tau}^{k,m} \in Z, \quad \varphi_i(s_{h\tau,i}^{k,m}) \in X_{\varphi_i(g_i)}, \quad i = 1, 2, \quad \Pi(s_{h\tau}^{k,m}, \cdot) \in X_{\Pi(g,\cdot)}. \quad (5.2)$$

This is a first crucial ingredient of our a posteriori error estimate and plays the role of the potential reconstruction in terms of [22]. It will be constructed cheaply, in an explicit way by local averaging.

- (iii) Define an *equilibrated flux reconstruction*  $\sigma_{h\tau}^{k,m}$  (in terms of [22]), piecewise constant in-time and  $\mathbf{H}(\text{div}, \Omega)$ -conforming, locally conservative on the mesh  $\mathcal{T}_h$ :

$$\sigma_h^{k,n,m} := \sigma_{h\tau}^{k,m}|_{\Gamma^n} \in \mathbf{RTN}_0(\Omega), \quad (5.3a)$$

$$\left( f^n - \frac{u_K^{k,n,m} - u_K^{k,n-1}}{\tau^n} - \nabla \cdot \sigma_h^{k,n,m}, 1 \right)_K = 0, \quad \forall K \in \mathcal{T}_h. \quad (5.3b)$$

This is again constructed cheaply, by a coarse problem on each time step followed by some local Neumann problems in bands close to the interface.

### 5.1 Postprocessed saturation $\tilde{u}_{h\tau}^{k,m}$

Consider an OSWR iteration  $k \geq 1$ , time step  $1 \leq n \leq N$ , and a linearization step  $m \geq 1$ . In each subdomain  $\Omega_i$ ,  $i = 1, 2$ , let  $\mathbf{u}_{h,i}^{k,n,m} \in \mathbf{RTN}_0(\Omega_i) \subset \mathbf{H}(\text{div}, \Omega_i)$  be prescribed by the fluxes  $F_{K,\sigma}(u_{h,i}^{k,n,m})$  of (4.1), i.e., on each  $K \in \mathcal{T}_{h,i}$  and each face  $\sigma \in \mathcal{E}_K$ ,

$$(\mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_i, 1)_\sigma = (F_{K,\sigma}(u_{h,i}^{k,n,m}), 1)_\sigma. \quad (5.4)$$

Extending [25, 22] to the present nonlinear context, we define the postprocessed approximation  $\tilde{\varphi}_{h,i}^{k,n,m} \in \mathbb{P}_2(\mathcal{T}_{h,i})$  in each element  $K \in \mathcal{T}_{h,i}$  as the solution of

$$-\nabla \tilde{\varphi}_{h,i}^{k,n,m}|_K = \mathbf{u}_{h,i}^{k,n,m}|_K, \quad \forall K \in \mathcal{T}_{h,i}, \quad (5.5a)$$

$$\frac{(\varphi_i^{-1}(\tilde{\varphi}_{h,i}^{k,n,m}), 1)_K}{|K|} = u_K^{k,n,m}, \quad \forall K \in \mathcal{T}_{h,i}. \quad (5.5b)$$

Procedure (5.5) is local in each mesh element and its cost is negligible. From  $\tilde{\varphi}_{h,i}^{k,n,m}$ , we construct the corresponding continuous, piecewise affine in-time postprocessed saturation by

$$\tilde{u}_{h\tau,i}^{k,m}(\cdot, t_n) = \tilde{u}_{h,i}^{k,n,m}, \quad 1 \leq n \leq N, \quad \text{where } \tilde{u}_{h,i}^{k,n,m} := \varphi_i^{-1}(\tilde{\varphi}_{h,i}^{k,n,m}). \quad (5.6)$$

Note that  $\tilde{u}_{h\tau}^{k,m}$  is nonconforming in the sense of (5.1).

**Remark 5.1** (Practice). *In practice, the condition (5.5b) will be approximated by a quadrature rule  $\tilde{\varphi}_{h,i}^{k,n,m}(\mathbf{x}_K) = \varphi_i(u_K^{k,n,m}) \forall K \in \mathcal{T}_{h,i}$ . Moreover, the postprocessed saturation  $\tilde{u}_{h,i}^{k,n,m}$  that involves  $\varphi_i^{-1}$  will only be used for the derivation of the estimates. In practice, the significant estimators in Theorem 6.1 below only involve the readily available  $\tilde{\varphi}_{h,i}^{k,n,m}$ , whereas those with  $\tilde{u}_{h,i}^{k,n,m}$  can be neglected. This is our main motivation for the proposed construction of the postprocessed saturation  $\tilde{u}_{h\tau}^{k,m}$ . Should one really need to calculate the estimators involving  $\tilde{u}_{h,i}^{k,n,m}$ , a practical approximation is to use corresponding quadrature rules and to let (5.6) (right) be satisfied in the quadrature nodes.*

### 5.2 Subdomain $H^1$ -conforming reconstruction $s_{h\tau}^{k,m}$

We define in this section the saturation reconstruction  $s_{h\tau}^{k,m}$ . It will belong to  $H^1(\Omega_i)$ ,  $i = 1, 2$ , and satisfy (5.2) (up to numerical quadrature). In contrast to the usual scenario, see [22, 38, 44], we cannot immediately apply the operator  $\mathcal{I}_{\text{av}}$  that prescribes averages in the Lagrange degrees of freedom to the postprocessed saturation  $\tilde{u}_{h\tau}^{k,m}$  constructed in section 5.1, since  $\tilde{u}_{h\tau}^{k,m}$  is generally a not a piecewise polynomial and, moreover, it is not constructed in practice, see Remark 5.1. Instead, we proceed in two steps.

First, from the available  $\tilde{\varphi}_{h,i}^{k,n,m} \in \mathbb{P}_2(\mathcal{T}_{h,i})$  defined by (5.5),  $k \geq 1$ ,  $1 \leq n \leq N$ ,  $m \geq 1$ , we define a piecewise polynomial that is continuous in each  $\Omega_i$  by

$$\hat{\varphi}_{h,i}^{k,n,m}(\mathbf{x}) := \mathcal{I}_{\text{av}}(\tilde{\varphi}_{h,i}^{k,n,m})(\mathbf{x}).$$

Here  $\mathbf{x}$  are the Lagrange degrees of freedom and  $\mathcal{I}_{\text{av}} : \mathbb{P}_2(\mathcal{T}_{h,i}) \rightarrow \mathbb{P}_2(\mathcal{T}_{h,i}) \cap H^1(\Omega_i)$  is the averaging operator given by

$$\mathcal{I}_{\text{av}}(\phi_h)(\mathbf{x}) = \frac{1}{|\mathcal{T}_{\mathbf{x}}|} \sum_{K \in \mathcal{T}_{\mathbf{x}}} \phi_h|_K(\mathbf{x}),$$

with  $\mathcal{T}_{\mathbf{x}}$  the set of all the elements of  $\mathcal{T}_{h,i}$  sharing the degree  $\mathbf{x}$  situated in the interior of  $\Omega_i$  or at the interface  $\Gamma$ . We set  $\hat{\varphi}_{h,i}^{k,n,m}(\mathbf{x}) := \varphi_i(g_i(\mathbf{x}))$  on the boundary  $\Gamma_i^{\text{D}}$ .

Second, we consider  $\varphi_i^{-1}(\hat{\varphi}_{h,i}^{k,n,m})$  in the Lagrange degrees of freedom to define  $s_h^{k,n,m}$ ; we modify it at the interface  $\Gamma$ , on the boundaries  $\Gamma_i^{\text{D}}$ , and in the element interiors to satisfy

$$\Pi_1(s_h^{k,n,m}|_{\Omega_1}) = \Pi_2(s_h^{k,n,m}|_{\Omega_2}) \text{ on } \Gamma, \quad (5.7a)$$

$$s_h^{k,n,m}|_{\Gamma_i^{\text{D}}} = g_i \text{ on } \Gamma_i^{\text{D}}, \quad i = 1, 2, \quad (5.7b)$$

$$\frac{1}{|K|} (s_h^{k,n,m}, 1)_K = u_K^{k,n,m}, \quad \forall K \in \mathcal{T}_h. \quad (5.7c)$$

Finally, the continuous piecewise affine in-time function  $s_{h\tau}^{k,m}$  is prescribed by

$$s_{h\tau}^{k,m}(\cdot, t_n) = s_h^{k,n,m}, \quad 1 \leq n \leq N. \quad (5.8)$$

**Remark 5.2** (Practice). *In practice, one can only satisfy condition (5.7a) in the sense of quadrature. Indeed, for  $1 \leq n \leq N$ ,  $1 \leq i \leq 2$ , any node  $\mathbf{x}_\Gamma$  of the chosen quadrature rule lying at the interface  $\Gamma$ , and  $j = (3 - i)$ , we can request*

$$\Pi_i(s_h^{k,n,m}|_{\Omega_i}(\mathbf{x}_\Gamma)) = \frac{\Pi_i(\varphi_i^{-1}(\hat{\varphi}_{h,i}^{k,n,m}(\mathbf{x}_\Gamma))) + \Pi_j(\varphi_j^{-1}(\hat{\varphi}_{h,j}^{k,n,m}(\mathbf{x}_\Gamma)))}{2}.$$

The last condition (5.7c) is easy to satisfy using the bubble functions following [22, Section 3.2.2], again up to a quadrature error.

### 5.3 Equilibrated flux reconstruction $\sigma_{h\tau}^{k,m}$

Because of the domain decomposition formulation with Robin or Ventcell transmission conditions, the finite volume fluxes  $F_{K,\sigma}(u_{h,i}^{k,n,m})$  of (4.1a) (or their linearizations  $F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m})$ ) of (4.5) do not match from the two sides of the interface  $\Gamma$ . Consequently,  $\mathbf{u}_h^{k,n,m}$  given by (5.4) is not  $\mathbf{H}(\text{div}, \Omega)$ -conforming (it does not lie in the space  $\mathbf{RTN}_0(\Omega)$ ), and cannot be used as a flux reconstruction in the sense of (5.3). To obtain  $\sigma_{h\tau}^{k,m}$ , the procedure used in the linear case in [4, 5] can be employed here. We relegate the details to Appendix A.

## 6 A posteriori error estimate

Relying on the developments of the previous sections, we derive here an a posteriori error estimate that bounds an energy error between the postprocessed saturation  $\tilde{u}_{h\tau}^{k,m}$  defined in section 5.1 and the weak solution  $u$  of Definition 2.2 by a guaranteed and fully computable upper bound, and this at each OSWR iteration  $k \geq 1$  and at each linearization step  $m \geq 1$ .

Recall the Poincaré inequality:

$$\|q - q_K\| \leq C_{P,K} h_K \|\nabla q\|_K, \quad \forall q \in H^1(K),$$

where  $q_K$  is the mean value of the function  $q$  on the element  $K$  and  $C_{P,K} = 1/\pi$  whenever the element  $K$  is convex. For all times  $t \in (0, T)$ , let also

$$Q_{t,i} := L^2(0, t; L^2(\Omega_i)), \quad X_t := L^2(0, t; H_0^1(\Omega)), \quad X'_t := L^2(0, t; H^{-1}(\Omega)).$$

Because of the assumptions on the weak solution  $u$  in Definition 2.2 and since, by (5.6),  $\varphi_i(\tilde{u}_{h\tau,i}^{k,m}) \in L^2(0, T; L^2(\Omega_i))$  for the postprocessed saturation  $\tilde{u}_{h\tau}^{k,m}$  defined in section 5.1,  $\tilde{u}_{h\tau}^{k,m} \in X'$ , and  $\tilde{u}_{h\tau}^{k,m}(\cdot, T) \in H^{-1}(\Omega)$ , we can define an energy-type error following [20] as

$$\begin{aligned} & \|u - \tilde{u}_{h\tau}^{k,m}\|_{\mathfrak{b}}^2 \\ & := \sum_{i=1}^2 \|\varphi_i(u_i) - \varphi_i(\tilde{u}_{h\tau,i}^{k,m})\|_{Q_{T,i}}^2 + \frac{L_\varphi}{2} \|u - \tilde{u}_{h\tau}^{k,m}\|_{X'}^2 + \frac{L_\varphi}{2} \|(u - \tilde{u}_{h\tau}^{k,m})(\cdot, T)\|_{H^{-1}(\Omega)}^2 \\ & \quad + 2 \sum_{i=1}^2 \int_0^T \left( \|\varphi_i(u_i) - \varphi_i(\tilde{u}_{h\tau,i}^{k,m})\|_{Q_{t,i}}^2 + \int_0^t \|\varphi_i(u_i) - \varphi_i(\tilde{u}_{h\tau,i}^{k,m})\|_{Q_{s,i}}^2 e^{t-s} ds \right) dt, \end{aligned} \quad (6.1)$$

where we recall that  $L_\varphi$  is the maximal Lipschitz constant of the functions  $\varphi_i$  defined by (2.7). We will also need the weaker distance

$$\begin{aligned} \|u - s_{h\tau}^{k,m}\|_{\mathfrak{b}} & := \sqrt{\frac{L_\varphi}{2}} \left\{ (2e^T - 1) \|u_0 - s_{h\tau}^{k,m}(\cdot, 0)\|_{H^{-1}(\Omega)}^2 + \|\mathcal{R}(s_{h\tau}^{k,m})\|_{X'}^2 \right. \\ & \quad \left. + 2 \int_0^T \left( \|\mathcal{R}(s_{h\tau}^{k,m})\|_{X'_t}^2 + \int_0^t \|\mathcal{R}(s_{h\tau}^{k,m})\|_{X'_s}^2 e^{t-s} ds \right) dt \right\}^{\frac{1}{2}} \end{aligned} \quad (6.2)$$

featuring the residual  $\mathcal{R}(s_{h\tau}^{k,m}) \in X'$  (recall the definition (2.11)) of the saturation reconstruction  $s_{h\tau}^{k,m}$  defined in section 5.2. This is given, for  $\psi \in X$ , by

$$\begin{aligned} & \langle \mathcal{R}(s_{h\tau}^{k,m}), \psi \rangle_{X',X} \\ & := \int_0^T \left\{ (f, \psi) - \langle \partial_t s_{h\tau}^{k,m}, \psi \rangle_{H^{-1}(\Omega), H_0^1(\Omega)} - \sum_{i=1}^2 (\nabla \varphi_i(s_{h\tau,i}^{k,m}), \nabla \psi)_{\Omega_i} \right\} (\theta) d\theta. \end{aligned} \quad (6.3)$$

Its dual norm on  $X'$  is then given by

$$\|\mathcal{R}(s_{h\tau}^{k,m})\|_{X'} := \sup_{\psi \in X, \|\psi\|_X=1} \langle \mathcal{R}(s_{h\tau}^{k,m}), \psi \rangle_{X',X}. \quad (6.4)$$

In (6.2), moreover,  $X'_t := L^2(0, t; H^{-1}(\Omega))$  and similarly for  $X'_s$ ,  $0 \leq s \leq t \leq T$ , with dual norms defined as in (6.4).

Our main result is summarized in the following theorem:

**Theorem 6.1** (A posteriori error estimate). *Let  $u$  be the weak solution of the multidomain problem (2.9)–(2.10) in the sense of Definition 2.2. Consider the Ventcell–OSWR algorithm (3.3)–(3.4) of section 3 on iteration  $k \geq 1$ , the finite volume discretization of section 4.2 on space and time meshes indexed by  $h$  and  $\tau$ , and the Newton linearization of section 4.3 on step  $m \geq 1$ . Let  $\tilde{u}_{h\tau}^{k,m}$  be the postprocessed saturation of section 5.1,  $s_{h\tau}^{k,m}$  the saturation reconstruction of section 5.2, and  $\sigma_{h\tau}^{k,m}$  the equilibrated flux reconstruction of section 5.3. Then*

$$\|u - s_{h\tau}^{k,m}\|_{\mathfrak{b}} \leq \eta^{k,m}. \quad (6.5)$$

Moreover, if

$$\bar{\varphi} \in X, \quad \text{where} \quad \bar{\varphi}|_{\Omega_i} := \varphi_i(u_i) - \varphi_i(s_{h\tau,i}^{k,m}), \quad i = 1, 2, \quad (6.6)$$

then

$$\|u - \tilde{u}_{h\tau}^{k,m}\|_{\mathfrak{H}} \leq \eta^{k,m} + \|\tilde{u}_{h\tau}^{k,m} - s_{h\tau}^{k,m}\|_{\mathfrak{H}}. \quad (6.7)$$

Here

$$\begin{aligned} \eta^{k,m} & := \sqrt{\frac{L_\varphi}{2}} \left\{ (2e^T - 1)(\eta_{\text{IC}}^{k,m})^2 + \sum_{n=1}^N (\eta^{k,n,m})^2 \right. \\ & \quad \left. + 2 \sum_{n=1}^N \tau^n \sum_{l=1}^n (\eta^{k,l,m})^2 + 2 \sum_{n=1}^N \sum_{l=1}^n J_{nl} \left( \sum_{q=1}^l (\eta^{k,q,m})^2 \right) \right\}^{\frac{1}{2}}, \end{aligned} \quad (6.8a)$$

where the initial condition estimator  $\eta_{\text{IC}}^{k,m}$  and the estimators  $\eta^{k,n,m}$  are respectively defined by

$$\eta_{\text{IC}}^{k,m} := \|u_0 - s_{h\tau}^{k,m}(\cdot, 0)\|_{H^{-1}(\Omega)}, \quad (6.8b)$$

$$\eta^{k,n,m} := \left\{ \int_{I^n} \sum_{i=1}^2 \sum_{K \in \mathcal{T}_{h,i}} \left( \eta_{\text{R},K}^{k,n,m} + \eta_{\text{disc},K,i}^{k,n,m}(t) \right)^2 dt \right\}^{\frac{1}{2}}, \quad 1 \leq n \leq N, \quad (6.8c)$$

the residual and the discretization estimators are respectively defined by

$$\eta_{\text{R},K}^{k,n,m} := C_{\text{P},K} h_K \|f^n - \partial_t s_{h\tau}^{k,m} - \nabla \cdot \sigma_h^{k,n,m}\|_K, \quad K \in \mathcal{T}_h, \quad (6.8d)$$

$$\eta_{\text{disc},K,i}^{k,n,m}(t) := \|\sigma_h^{k,n,m} + \nabla \varphi_i(s_{h\tau}^{k,m}(\cdot, t))\|_K, \quad K \in \mathcal{T}_{h,i}, \quad t \in I^n, \quad (6.8e)$$

and where we have set, for  $1 \leq n, l \leq N$ ,

$$J_{nl} := \int_{I^n} \int_{I^l} e^{t-s} ds dt.$$

*Proof.* We have set  $s_{h\tau}^{k,m}$  so that  $\varphi_i(s_{h\tau}^{k,m}) \in X_{\varphi_i(g_i)}$ ,  $\Pi(s_{h\tau}^{k,m}, \cdot) \in X_{\Pi(g, \cdot)}$ , and

$$(f^n - \partial_t s_{h\tau}^{k,m}|_{I^n} - \nabla \cdot \boldsymbol{\sigma}_h^{k,n,m}, 1)_K = 0 \quad \forall K \in \mathcal{T}_h, 1 \leq n \leq N. \quad (6.9)$$

Indeed, (6.9) follows from the requirement (5.7c) which implies

$$(\partial_t s_{h\tau}^{k,m}|_{I^n}, 1)_K = \left( \frac{s_h^{k,n,m} - s_h^{k,n-1}}{\tau^n}, 1 \right)_K = \left( \frac{u_K^{k,n,m} - u_K^{k,n-1}}{\tau^n}, 1 \right)_K$$

together with (5.3b). Thus, adding and subtracting  $(\boldsymbol{\sigma}_{h\tau}^{k,m}, \nabla \psi)$  in (6.3) and using the Green theorem and the fact that  $\partial_t s_{h\tau}^{k,m} \in L^2(0, T; L^2(\Omega))$ , we infer

$$\begin{aligned} & \langle \mathcal{R}(s_{h\tau}^{k,m}), \psi \rangle_{X', X} \\ &= \sum_{n=1}^N \int_{I^n} \left\{ (f - \partial_t s_{h\tau}^{k,m} - \nabla \cdot \boldsymbol{\sigma}_h^{k,n,m}, \psi) - \sum_{i=1}^2 (\nabla \varphi_i(s_{h\tau}^{k,m}) + \boldsymbol{\sigma}_h^{k,n,m}, \nabla \psi)_{\Omega_i} \right\} (\theta) d\theta. \end{aligned}$$

From (6.4) and using (6.9), it then immediately follows that

$$\|\mathcal{R}(s_{h\tau}^{k,m})\|_{X'}^2 \leq \sum_{n=1}^N (\eta^{k,n,m})^2.$$

Proceeding as in [20, Theorem 5.3], we then promptly arrive at (6.5). Next, it follows by inspection of the proof of [20, Theorem 5.2] that, under assumption (6.6), we have

$$\|u - s_{h\tau}^{k,m}\|_{\#} \leq \|u - s_{h\tau}^{k,m}\|_b. \quad (6.10)$$

Thus (6.7) follows by the triangle inequality

$$\|u - \tilde{u}_{h\tau}^{k,m}\|_{\#} \leq \|u - s_{h\tau}^{k,m}\|_{\#} + \|\tilde{u}_{h\tau}^{k,m} - s_{h\tau}^{k,m}\|_{\#}.$$

□

**Remark 6.2** (Condition (6.6)). *Condition (6.6) seems unfortunately necessary to apply [20, Theorem 5.2] so as to obtain (6.10) and consequently the a posteriori estimate (6.7). It is indeed rather restrictive for the complete problem (2.9)–(2.10). It is, though, in particular satisfied when the global mobilities of the gas  $\lambda_i$  are constants in the respective subdomains  $\Omega_i$  and  $\pi_1(0) = \pi_2(0)$ . In this case, we get an estimate in the norm  $\|\cdot\|_{\#}$  defined by (6.1) for the present nonlinear degenerate parabolic problem, where the transmission conditions are nonlinear and indeed discontinuous, since  $\bar{\pi}_1(u_1) = \bar{\pi}_2(u_2)$  but  $u_1 \neq u_2$  in general at the interface  $\Gamma$ . In general, when condition (6.6) is not satisfied, we only control the dual residual norm  $\|\cdot\|_b$  defined by (6.2).*

**Remark 6.3** (A posteriori estimate of the saturation and capillary pressure errors). *Applying (2.8), the above estimators bound also the saturation and the capillary pressure errors. More precisely, replacing the functions  $\varphi_i$  by the functions  $\Pi_i$  in (6.1), the estimate (6.7) still holds.*

## 7 Distinguishing the space, time, linearization, and the DD errors

In this section, we distinguish the different error components, proceeding as in [23, 17, 20, 5] and the references therein. The aim is in particular to separate the domain decomposition error from the estimated space, time, and linearization errors.

For the iteration  $k \geq 1$  of the OSWR algorithm, for all time steps  $0 \leq n \leq N$ , a linearization step  $m \geq 1$ , and both subdomains  $\Omega_i$ ,  $i = 1, 2$ , we define a vector function  $\boldsymbol{\ell}_{h,i}^{k,n,m} \in \mathbf{RTN}(\Omega_i)$  that approximates the available flux used in the Newton iterations in section 4.3, i.e.,

$$(\boldsymbol{\ell}_{h,i}^{k,n,m} \cdot \mathbf{n}_i, 1)_{\sigma} = (F_{K,\sigma}^{m-1}(u_{h,i}^{k,n,m}), 1)_{\sigma}, \quad \forall \sigma \in \mathcal{E}_K, \forall K \in \mathcal{T}_{h,i}. \quad (7.1)$$



The vector function  $\boldsymbol{\ell}_{h,i}^{k,n,m}$  is called the linearized flux. It tends to  $\mathbf{u}_{h,i}^{k,n,m}$  defined in (5.4) at convergence of the Newton algorithm. For all  $K \in \mathcal{T}_{h,i}$ , we then define the local *spatial*, *temporal*, *domain decomposition*, and *linearization* estimators by:

$$\eta_{\text{sp},K,i}^{k,n,m} := \eta_{\text{R},K}^{k,n,m} + \|\nabla \varphi_i(s_{h\tau}^{k,m}(\cdot, t_n)) + \boldsymbol{\ell}_{h,i}^{k,n,m}\|_K, \quad (7.2a)$$

$$\eta_{\text{tm},K,i}^{k,n,m}(t) := \|\nabla(\varphi_i(s_{h\tau}^{k,m}(\cdot, t)) - \varphi_i(s_{h\tau}^{k,m}(\cdot, t_n)))\|_K, \quad (7.2b)$$

$$\eta_{\text{dd},K,i}^{k,n,m} := \|\mathbf{u}_{h,i}^{k,n,m} - \boldsymbol{\sigma}_h^{k,n,m}\|_K, \quad (7.2c)$$

$$\eta_{\text{lin},K,i}^{k,n,m} := \|\mathbf{u}_{h,i}^{k,n,m} - \boldsymbol{\ell}_{h,i}^{k,n,m}\|_K. \quad (7.2d)$$

Note that (7.2c) and (7.2d) only work with lowest-order Raviart–Thomas–Nédélec polynomials, so that they can be evaluated without numerical quadrature error and fast. Note also that from (5.6) and (5.5a), actually  $\mathbf{u}_{h,i}^{k,n,m} = -\nabla \varphi_i(\tilde{u}_{h,i}^{k,n,m})$ . Set, like in (6.8c), for  $a = \text{sp}, \text{tm}, \text{dd}, \text{lin}$ ,

$$(\eta_{a,i}^{k,n,m})^2 := \int_{I^n} \sum_{K \in \mathcal{T}_{h,i}} (\eta_{a,K,i}^{k,n,m})^2 dt \quad \text{and} \quad (\eta_a^{k,n,m})^2 := \sum_{i=1}^2 (\eta_{a,i}^{k,n,m})^2, \quad (7.3)$$

and note that except for  $a = \text{tm}$ ,  $(\eta_{a,i}^{k,n,m})^2 = \tau^n \sum_{K \in \mathcal{T}_{h,i}} (\eta_{a,K,i}^{k,n,m})^2$ ; for  $a = \text{tm}$ , the dependence of the estimators on time is left implicit. The global versions, like in (6.8a) but without the initial condition, are

$$\begin{aligned} \eta_a^{k,m} := & \sqrt{\frac{L_\varphi}{2}} \left( \left\{ \sum_{n=1}^N (\eta_a^{k,n,m})^2 \right\}^{\frac{1}{2}} + \sqrt{2} \left\{ \sum_{n=1}^N \tau^n \sum_{l=1}^n (\eta_a^{k,l,m})^2 \right\}^{\frac{1}{2}} \right. \\ & \left. + \sqrt{2} \left\{ \sum_{n=1}^N \sum_{l=1}^n J_{nl} \sum_{q=1}^l (\eta_a^{k,q,m})^2 \right\}^{\frac{1}{2}} \right) + \delta_a \|\tilde{u}_{h\tau}^{k,m} - s_{h\tau}^{k,m}\|_{\sharp}, \end{aligned} \quad (7.4)$$

where  $\delta_a = 0$  for  $a = \text{tm}, \text{dd}, \text{lin}$  and  $\delta_{\text{sp}}$  will take the values 0 or 1, depending on the norm in which the error is measured. Then using estimates (6.7) and (6.5) together with the triangle inequality gives:

**corollary 7.1** (A posteriori error estimate distinguishing error components). *Let the assumptions of Theorem 6.1 be satisfied. Let the linearized flux  $\boldsymbol{\ell}_h^{k,n,m}$  be given by (7.1) and the estimators by (6.8b) and (7.2)–(7.4). Then, with  $\delta_{\text{sp}} = 0$ ,*

$$\|u - s_{h\tau}^{k,m}\|_{\flat} \leq \sqrt{\frac{L_\varphi}{2}} \sqrt{2e^T - 1} \eta_{\text{IC}}^{k,m} + \eta_{\text{sp}}^{k,m} + \eta_{\text{tm}}^{k,m} + \eta_{\text{dd}}^{k,m} + \eta_{\text{lin}}^{k,m},$$

and, under condition (6.6) and with  $\delta_{\text{sp}} = 1$ ,

$$\|u - \tilde{u}_{h\tau}^{k,m}\|_{\sharp} \leq \sqrt{\frac{L_\varphi}{2}} \sqrt{2e^T - 1} \eta_{\text{IC}}^{k,m} + \eta_{\text{sp}}^{k,m} + \eta_{\text{tm}}^{k,m} + \eta_{\text{dd}}^{k,m} + \eta_{\text{lin}}^{k,m}.$$

## 8 Stopping criteria and optimal balancing of the different error components

We provide here stopping criteria for the OSWR algorithm and the nonlinear solver for the subdomain problems as in [23, 17, 20, 5] and the references therein. The goal is to efficiently use the computer resources while saving many unnecessary iterations and to equilibrate all error components.

Let two real parameters  $\delta_{\text{lin}}$  and  $\delta_{\text{dd}}$  be given in  $(0, 1)$ . The stopping criteria for the linearization step (inner loop in  $m$ ) in each subdomain  $i$ , at each time step  $n$ , and each OSWR iteration  $k$  is chosen as, employing the estimates (7.3)

$$\eta_{\text{lin},i}^{k,n,m} \leq \delta_{\text{lin}} \max \left\{ \eta_{\text{sp},i}^{k,n,m}, \eta_{\text{tm},i}^{k,n,m}, \eta_{\text{dd},i}^{k,n,m} \right\}, \quad i = 1, 2. \quad (8.1)$$

Similarly, the stopping criteria for the OSWR algorithm (outer loop in  $k$ ) is set as, employing the estimates (7.4),

$$\eta_{\text{dd}}^{k,m} \leq \delta_{\text{dd}} \max \left\{ \eta_{\text{sp}}^{k,m}, \eta_{\text{tm}}^{k,m} \right\}. \quad (8.2)$$

The first criterion (8.1) stipulates that there is no need to continue with the linearization iterations if the overall error is dominated by the other components. That of the second criterion (8.2) decides that we stop the OSWR algorithm if the domain decomposition error is dominated by one of the other components. The entire procedure of the approach is then described by the following adaptive algorithm:

**Data:**  $T, u_0, \Omega_i, \pi_i, \lambda_i, g_i,$  and  $f_i, i = 1, 2.$

**Result:** The saturations  $u_{h\tau}^{k,m}$ .

```

1:  $k := 0$ 
2: repeat
3:    $k := k + 1$ 
4:   for  $i=1,2$  do
5:      $j := 3 - i; n := 0$ 
6:     while  $t^n \leq T$  do
7:        $n := n + 1; m := 0$ 
8:       repeat
9:          $m := m + 1$ 
10:         $u_{h,i}^{k,n,m} := \Upsilon_i(u_{h,i}^{k,n,m-1}, \Psi_j^{k-1,n}, f_i^n, u_{h,i}^{k,n-1})$  by (4.4)
11:        Compute  $\eta_{\text{sp},i}^{k,n,m}, \eta_{\text{tm},i}^{k,n,m}, \eta_{\text{dd},i}^{k,n,m},$  and  $\eta_{\text{lin},i}^{k,n,m};$ 
12:        until  $\eta_{\text{lin},i}^{k,n,m} \leq \delta_{\text{lin}} \max \left\{ \eta_{\text{sp},i}^{k,n,m}, \eta_{\text{tm},i}^{k,n,m}, \eta_{\text{dd},i}^{k,n,m} \right\}$ 
13:         $u_{h,i}^{k,n} := u_{h,i}^{k,n,m};$ 
14:         $\Psi_i^{k-1,n} := \{ \Psi_{L,\sigma}^{k-1,n} \}_{\sigma=K|L, K \in \mathcal{T}_{h,i}, L \in \mathcal{T}_{h,j}}$  by (4.3)
15:      end while
16:    end for
17:    Compute  $\eta_{\text{sp}}^{k,m}, \eta_{\text{tm}}^{k,m}, \eta_{\text{dd}}^{k,m}$ 
18:  until  $\eta_{\text{dd}}^{k,m} \leq \delta_{\text{dd}} \max \left\{ \eta_{\text{sp}}^{k,m}, \eta_{\text{tm}}^{k,m} \right\}$ 

```

**Algorithm 1:** Complete solution algorithm with adaptive stopping criteria

**Remark 8.1** (Space and time adaptivity). *The above local-in-time estimators are calculated on each element of the mesh and on each time step, and could also be used as indicators in order to refine adaptively the time steps  $\tau^n$  and/or the space meshes  $\mathcal{T}_{h,i}$ , see [20, 17, 44] and the references therein.*

## 9 Numerical experiments

In this section we illustrate the efficiency of our theoretical results on numerical experiments.

We have chosen three examples designed to show how the method behaves in various physical and geometrical situations.

- The first example is a simple academic situation (coming from [21]), which already contains the main difficulty, i.e., a discontinuous capillary pressure function. It is chosen to demonstrate the features of the method.
- The second example (from [30]) models the infiltration of a dense non-aqueous phase liquid (DNAPL) in a low-capillarity lens, and involves a geometrically more complex interface that acts as a “capillarity trap”.
- In the last example shown (taken from [3]), the flow is tangential to the interface, which may render the application of a DD method more delicate. Furthermore, the capillary pressure function is of a form widely used for two-phase flow simulations (Van Genuchten model).

## 9.1 Example 1: two rock types with a straight interface

In a three-dimensional extension of an example from [21], take  $\Omega = [0, 1]^3$  and  $T = 15$ . The subdomains are  $\Omega_1 = \{0 < x < 1/2\}$  and  $\Omega_2 = \{1/2 < x < 1\}$ , with  $\Gamma = \{x = 1/2\}$ . The capillary pressure functions and the global mobilities are given respectively by

$$\pi_1(u) = 5u^2, \quad \pi_2(u) = 5u^2 + 1, \quad \lambda_i(u) = u(1 - u), \quad i \in \{1, 2\}. \quad (9.1)$$

We impose Dirichlet conditions on two subsets of the boundary  $\partial\Omega$ . The saturation is set equal to 0.9 on  $\Gamma_{D,\text{in}} = \{(x, y, z) \in \partial\Omega \mid x = 0 \text{ and } 0.4 \leq y \leq 0.6\}$ . On the outflow boundary  $\Gamma_{\text{out}} = \{(x, y, z) \in \partial\Omega \mid x = 1\}$ , the saturation at time  $t^{n+1}$  is set equal to that inside the closest cell at time  $t^n$  (see [1]). We assume homogeneous Neumann boundary conditions on the remaining part of the boundary. The initial condition is taken to be zero everywhere, which satisfies (2.6a) and consequently (2.10a) at the interface between the rocks. We take  $f = 0$  in  $\Omega_1$  and  $\Omega_2$ . The gas has to go through subdomain  $\Omega_1$  before entering subdomain  $\Omega_2$ . Note that the gas cannot enter the subdomain  $\Omega_2$  as long as the capillary pressure  $\pi_1(u_1)$  remains lower than the entry pressure  $\pi_1(u_1^*)$ , with  $u_1^* = \frac{1}{\sqrt{5}}$ .

For the spatial discretization we use uniform meshes in the subdomains, consisting of rectangular parallelepipeds matching on the interface  $\Gamma$ . The implementation is based on the MATLAB Reservoir Simulation Toolbox [35], and makes use of its automatic differentiation feature to compute the Jacobian matrices for solving the nonlinear subdomain problems by the Newton method. The optimized (Robin or Ventcell) parameters are computed by numerically minimizing the continuous convergence factor corresponding to a linearized version of the problem (see [2] for details).

In the rest of this section, we denote the method defined by using the OSWR method with Robin transmission conditions by Robin–OSWR, while the method using full Ventcell transmission conditions will be denoted by Ventcell–OSWR. When appropriate, we qualify the Robin conditions as one-sided ( $\alpha_{12} = \alpha_{21}$ ) or two-sided in the more general case.

### 9.1.1 The performance of the OSWR method with adaptive stopping criteria

We first consider the OSWR algorithm with one-sided Robin transmission conditions in (3.2), i.e.  $\gamma_{12} = \gamma_{21} = 0$  and  $\alpha = \alpha_{1,2} = \alpha_{2,1}$ . Two snapshots of the saturation are shown in Fig. 3, together with two snapshots of the capillary pressure in Fig. 4. As expected, both the saturation of the gas in  $\Omega_1$  and the capillary pressure increase until the capillary pressure reaches the entry pressure. It can be seen that the capillary pressure field becomes continuous when the entry pressure is reached, then  $\Omega_2$  is infiltrated by the gas, but the saturation remains discontinuous across the interface and some quantity of gas remains trapped under the rock discontinuity.

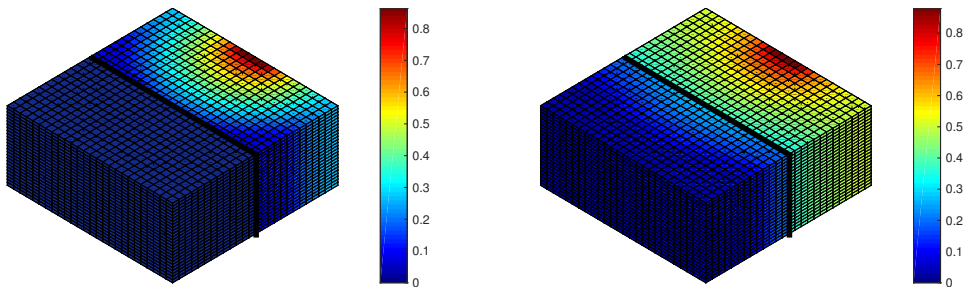
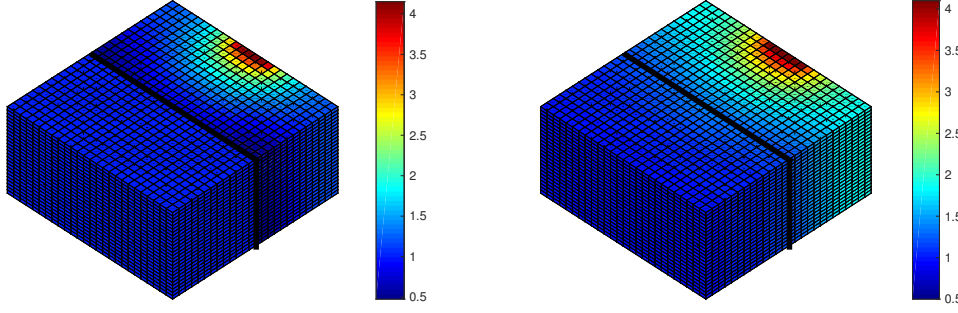


Figure 3: Test case 1: Robin interface conditions, saturation  $u(t)$  for  $t = 6.6$  and  $t = 15$

Next we assess the performance of the optimized parameter  $\alpha$  of our Robin–OSWR algorithm of section 3. Fig. 5 (left) shows the domain decomposition estimator  $\eta_{\text{dd}}^{k,m}$  (defined in (7.2)–(7.4)) after 25 OSWR iterations as a function of  $\alpha$ . The estimator behaves very similarly to what is usually observed for the DD error (see, e.g., [26]). Moreover, the optimized parameter (marked by a square) is close to the numerically optimal value. This result points the way to the possibility of finding the optimal Robin parameter by minimizing the DD estimator  $\eta_{\text{dd}}^{k,m}$ . It also confirms the ability of the DD estimator to separate the domain decomposition error from the other components of the global error.


Figure 4: Test case 1: Robin interface conditions, capillary pressure  $\pi(u(t), \cdot)$  for  $t = 6.6$  and  $t = 15$ 

We now analyze the performance of the adaptive stopping criteria (8.2) described in section 8. In particular, we compare them with the common approach in which the OSWR algorithm is continued until the relative Robin residual in  $L^2$ -norm on the space-time interface  $\Gamma \times (0, T)$  becomes smaller than a threshold taken as  $10^{-6}$ , i.e.,

$$\text{err}_{\text{OSWR}}^k := \left( \frac{\sum_{i=1}^2 \sum_{n=1}^N \|\Psi_i^{k,n} - \Psi_i^{k-1,n}\|_{L^2(\Gamma)}^2}{\sum_{i=1}^2 \sum_{n=1}^N \|\Psi_i^{k-1,n}\|_{L^2(\Gamma)}^2} \right)^{\frac{1}{2}} \leq 10^{-6}. \quad (9.2)$$

The Newton iterations are stopped when the residuals in both subdomains  $\Omega_i$  satisfy

$$\text{err}_{\text{lin},i}^{k,n,m} := \frac{\|\varphi_i(u_{h,i}^{k,n,m}) - \varphi_i(u_{h,i}^{k,n,m-1})\|_{\infty, \Omega_i}}{\|\varphi_i(u_{h,i}^{k,n,m-1})\|_{\infty, \Omega_i}} \leq 10^{-8}. \quad (9.3)$$

In Fig. 5 (right), we plot the different estimators as functions of the OSWR iterations. The adaptive stopping criterion (8.2) needs only 10 iterations, while the classical stopping criterion (9.2) requires 21 iterations.

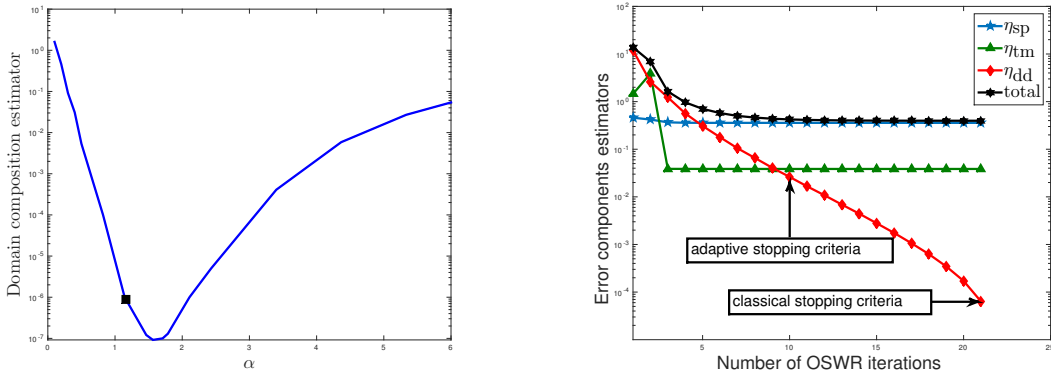
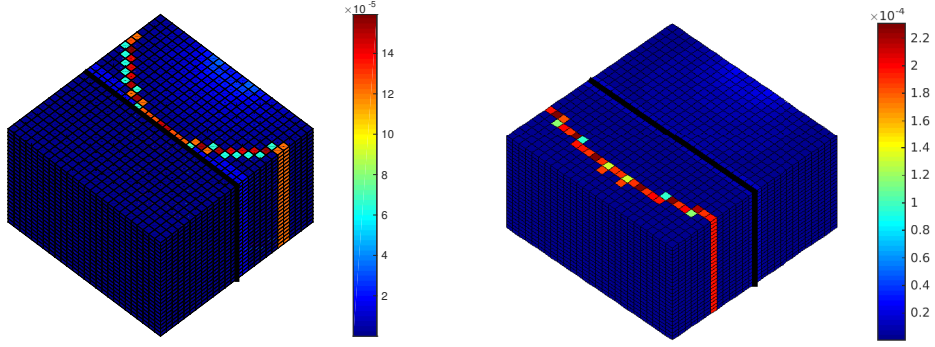
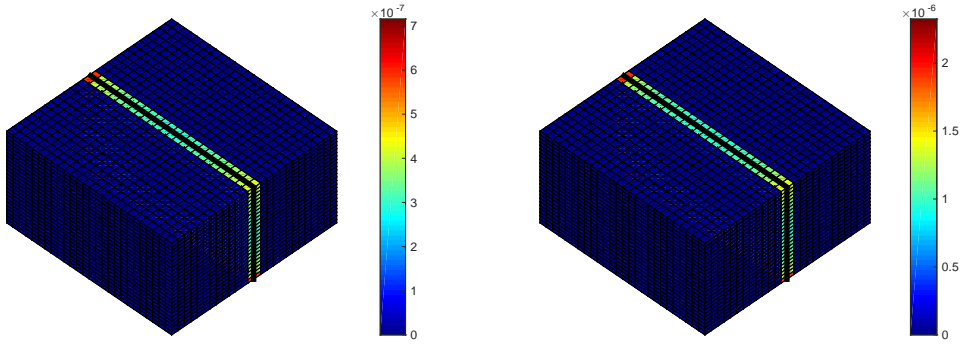

Figure 5: Test case 1: Domain decomposition estimator  $\eta_{\text{dd}}^{k,m}$  after 25 Robin-OSWR iterations as a function of the parameter  $\alpha$  (left) and evolution of the spatial, temporal, and domain decomposition estimators as a function of the number of Robin-OSWR iterations until  $\text{err}_{\text{OSWR}}^{21} \leq 10^{-6}$  (right)

Fig. 6 next depicts the evolution of the estimated error after using the stopping criteria (8.2) with  $\delta_{\text{dd}} = 0.1$  and (8.1) with  $\delta_{\text{lin}} = 0.1$ . We notice that the error distribution follows the saturation front but also that some error can still be detected near the interface. In Fig. 7, the domain decomposition error is shown at two different time steps, and clearly one can remark that the DD error is not affecting the global error, in agreement with (8.2).

Fig. 8 finally plots the different estimators in each subdomain, as a function of the Newton iteration at the final iteration of the OSWR algorithm. Only three iterations are required to reach (8.1) for the subdomain solvers, while 9 iterations for the solves in  $\Omega_1$  and 6 in  $\Omega_2$  are needed to reach the classical criteria (9.3).


Figure 6: Test case 1: Robin interface conditions, estimated global error for  $t = 6.6$  and  $t = 15$ 

Figure 7: Test case 1: Robin interface conditions, estimated DD error for  $t = 6.6$  and  $t = 15$ 

### 9.1.2 Comparison of the Robin– and Ventcell–OSWR algorithms with adaptive stopping criteria

We now consider the OSWR algorithm with the two-sided Robin transmission conditions (i.e.  $\gamma_{12} = \gamma_{21} = 0$  and  $\alpha_{12} \neq \alpha_{21}$ ) on the one hand, and the Ventcell transmission conditions (i.e.  $\gamma = \gamma_{12} = \gamma_{21}$  and  $\alpha = \alpha_2 = \alpha_{21}$ ) on the other hand. Fig. 9 shows, for each method, the different estimators as a function of the number of DD iterations. We observe that the estimated space and time errors coincide for the two methods and that they are also very close to those obtained with the one-sided Robin–OSWR algorithm (see Fig. 5), as expected. For the DD error, both methods are faster than the one-sided Robin–OSWR method. The usual stopping criteria are reached after 10 and 7 iterations, respectively, whereas only 4 iterations are needed with the adaptive stopping criteria (8.2). Fig. 10 shows contour lines of the DD estimator  $\eta_{\text{dd}}^{k,m}$  as a function of the parameters, at the final OSWR iteration. The square marks the parameters obtained via the optimization procedure described at the beginning of this section. The square corresponds also to  $\text{err}_{\text{OSWR}}^4 \approx 1.9 \cdot 10^{-3}$  for the Robin–OSWR method and  $\text{err}_{\text{OSWR}}^3 \approx 2.15 \cdot 10^{-4}$  for the Ventcell–OSWR method. It is worth noting that this optimized parameter is close to the parameter that numerically minimizes the error estimate  $\eta_{\text{dd}}^{k,m}$ .

We have also checked the efficiency of the adaptive linearization stopping criterion (8.1) for both methods. The results (not shown here) are similar to the Robin–OSWR case, which allows to stop the Newton algorithm after 4 iterations for most of the solves, instead of 7–10 and 11–14, respectively, for the classical criterion (9.3).

## 9.2 DNAPL infiltration in a low capillarity lens

We consider a DNAPL infiltration problem with two different rock types, inspired from [30]. We take  $\Omega = [0, 1]^3$  and  $T = 4 \cdot 10^2$ . The medium contains a lens with different capillary pressure curve. The gas and water mobilities depend only on space and are given by  $\lambda_1(u) = 1/4$ ,  $\lambda_2(u) = 2/3$ , and the capillary pressure curves have the form (see Fig. 11)

$$\pi_1(u) = -\ln(1-u), \quad \text{and} \quad \pi_2(u) = -(0.5 + \ln(1-u)).$$

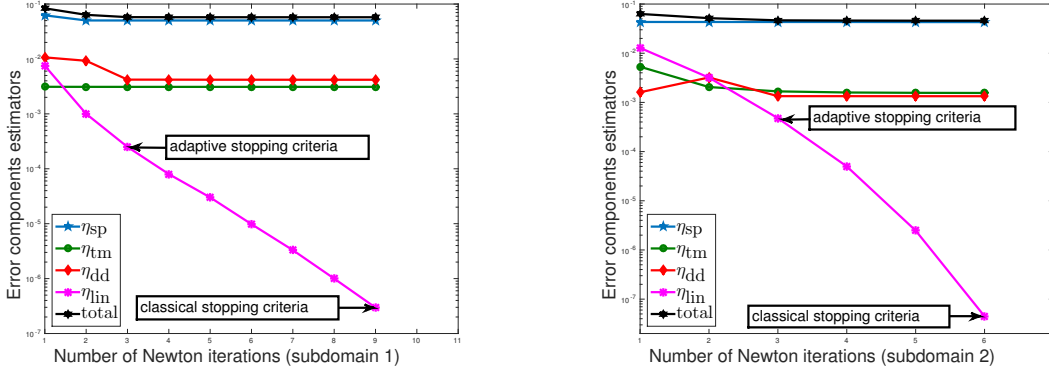


Figure 8: Test case 1: Robin interface conditions, evolution of the spatial, temporal, domain decomposition, and linearization error estimators as a function of Newton iterations for the final iteration of OSWR algorithm for  $t = 6.6$ ; subdomain 1 (left) and subdomain 2 (right)

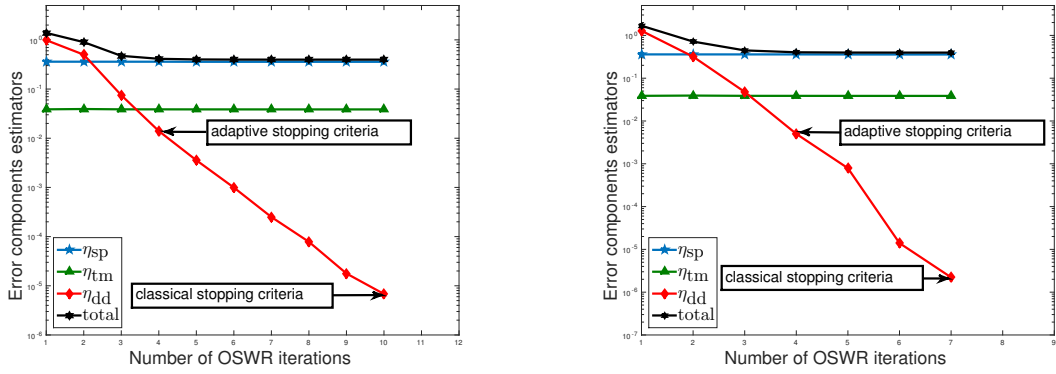


Figure 9: Test case 1: Spatial, temporal, and domain decomposition error estimators as a function of OSWR iterations for the two-sided Robin-OSWR method (left) and the Ventcell-OSWR method (right)

The gas is injected along one side of the domain and a Dirichlet condition is imposed on the opposite face, while no-flow boundary conditions are imposed on the remaining faces. We use a uniform mesh with 17576 elements (corresponding to 26 elements in each layer of each direction).

The time interval  $[0, T]$  is decomposed into 8 equal time windows. The OSWR algorithm is employed over each time window until the stopping criteria (8.2) is satisfied, and then the next time window is treated by the DD algorithm. For this example, we use the 2-sided Robin-OSWR method. The Robin parameters are calculated using the same procedure as in the first test case for the first time window, and we keep the same optimized parameters for all time windows.

Fig. 12 shows the evolution of the saturation over the whole domain. In this experiment, the flow is driven by the difference in the capillary pressures. In contrast to the previous test case, when the gas reaches the interface, the flow crosses immediately the interface through the domain  $\Omega_2$  and the gas accumulates into the lens as the capillary pressure remains discontinuous. The gas inside rock type 2 snakes around the interface to travel again through rock type 1 and then starts to spread into the surrounding medium when the entry pressure given by  $\pi_1(0) = 0$  is reached. In fact, the lens acts as a capillary trap as it is much easier for the gas to enter the lens than to leave it, because of the difference in capillary pressures.

We come now to the analysis of the OSWR algorithm. In Fig. 13, we plot the different estimators as functions of the OSWR iterations for the first, fifth, and final time windows. The classical OSWR algorithm needs 49 iterations overall to converge, with 7 iterations for the first time window, and then between 5

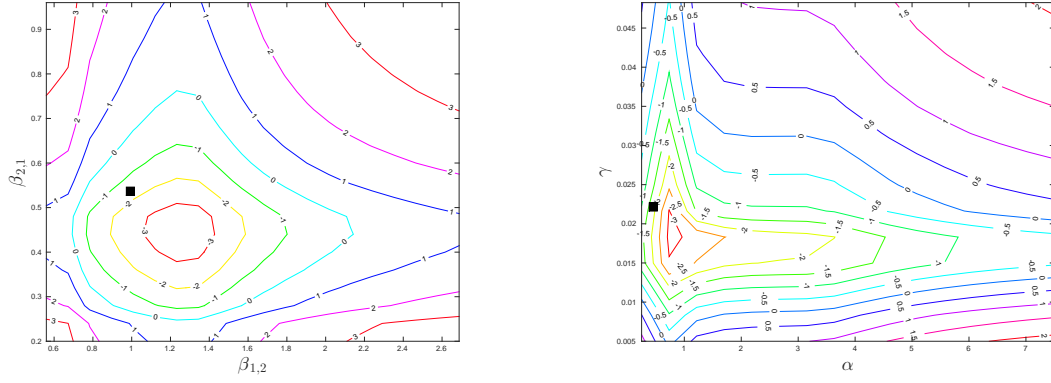


Figure 10: Test case 1: Domain decomposition error estimator  $\eta_{\text{dd}}^{k,m}$  as a function of the free parameters after 4 iterations of the OSWR of the two-sided Robin-OSWR method (left) and 3 iterations of the optimized Ventcell-OSWR method (right)

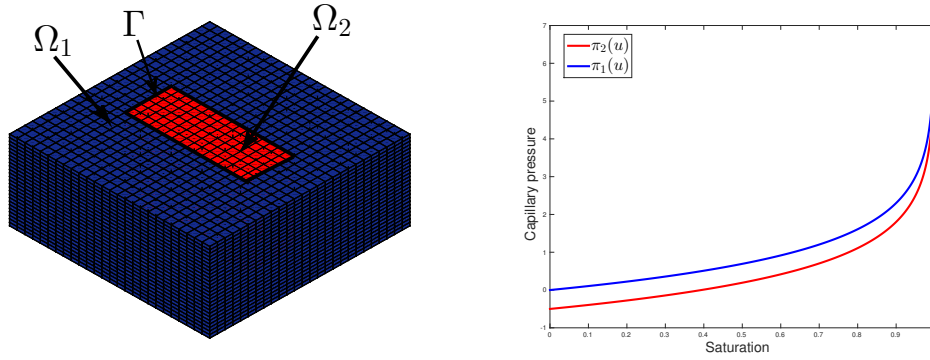


Figure 11: Test case 2: geometry and mesh (left), capillary pressure functions (right)

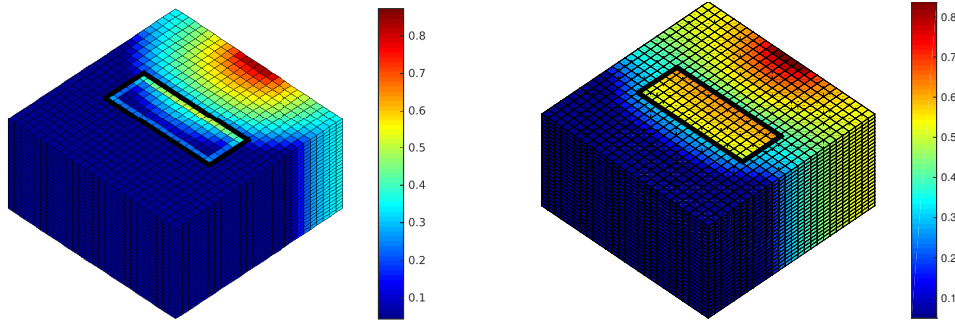


Figure 12: Test case 2: saturation, for  $t = 1.5 \cdot 10^2$  and  $t = 4 \cdot 10^2$

and 7 iterations for the remaining ones. The adaptive OSWR needs 5 iterations to reach the DD stopping criteria for the first time window, and then 2 or 3 iterations for the remaining ones, see Fig 14 (left) for the details, and 24 in total. The adaptive linearization stopping criterion (8.1) is also an efficient way of stopping the Newton iterations. In Fig. 14 (right), we plot the cumulative number of Newton iterations for the last OSWR iteration. In average, the adaptive stopping criteria reduce the number of Newton iterations from 15.9 to 8.3.

In Fig. 15, we plot the evolution of the estimates, using the stopping criteria (8.2) with  $\delta_{\text{dd}} = 0.1$  and (8.1) with  $\delta_{\text{lin}} = 0.1$ . As for the previous test case, again the distribution follows the saturation front

and also renders some error near the interface.

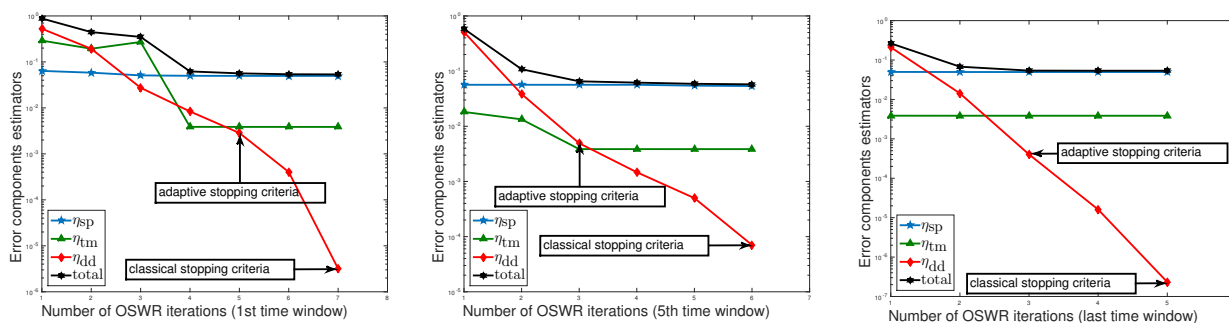


Figure 13: Test case 2: evolution of the spatial, temporal, and domain decomposition error estimators as a function of the number of Robin–OSWR iterations for the first (left), fifth (middle), and last (right) time windows

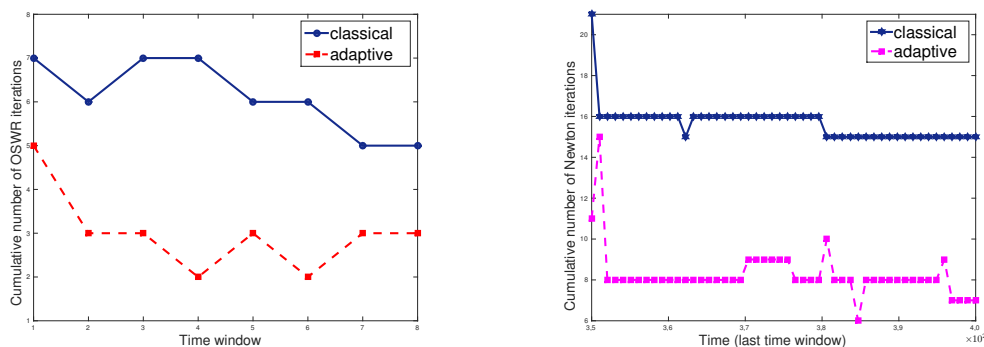


Figure 14: Test case 2: The cumulative number of OSWR iterations as a function of time windows (left) and the cumulative number of Newton iterations for the last OSWR iteration (last window) as a function of time (right)

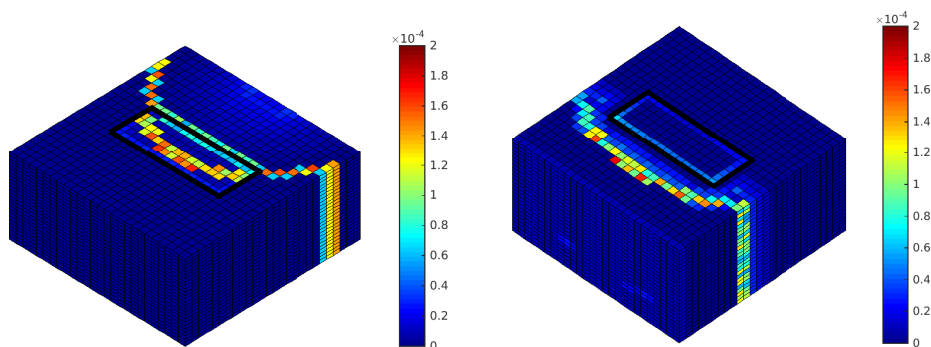


Figure 15: Test case 2: estimated error for  $t = 1.5 \cdot 10^2$  and  $t = 4 \cdot 10^2$

### 9.3 Test case 3: injection along a discontinuity

We consider a numerical experiment from [3] given by the displacement of a non-wetting fluid by a wetting fluid in a domain made up of two regions with different rock types. The domain is taken as  $\Omega = [0, 10]^3$



and the final time is  $T = 400$ . The injection boundary is taken orthogonal to the interface  $\Gamma$  which makes the flow parallel to the discontinuity and compete in the two subdomains to reach the production boundary on the opposite side. In this example, the capillary pressure functions and the mobilities are given by the widely used Van Genuchten model [43], i.e.,

$$\pi_i(u) = P_i((1-u)^{-1/\mu} - 1)^{1/\nu}, \quad \text{and} \quad \lambda_i = \frac{\lambda_w(u)\lambda_n(u)}{\lambda_w(u) + \lambda_n(u)}$$

, where  $\lambda_w(u)$  and  $\lambda_n(u)$  are the phase mobilities

$$\lambda_w(u) = \sqrt{u}[1 - (1 - u^\nu)^\mu]^2, \quad \text{and} \quad \lambda_n(u) = (1 - u)^2(1 - u^\nu)^{2\mu},$$

with  $\nu = 2.8$ ,  $\mu = 1 - 1/\nu$ , and  $P_1$  and  $P_2$  two constants depending on the rock parameters. We take  $P_1 = 10$  and  $P_2 = 5$ . Implicitly, this choice implies that rock type 1 is two times more permeable than rock type 2. Contrarily to the previous test cases, the capillary pressure functions are now matching between the two rock types, see Fig. 16 (left) (cf. also condition (2.3) and Remark 6.2).

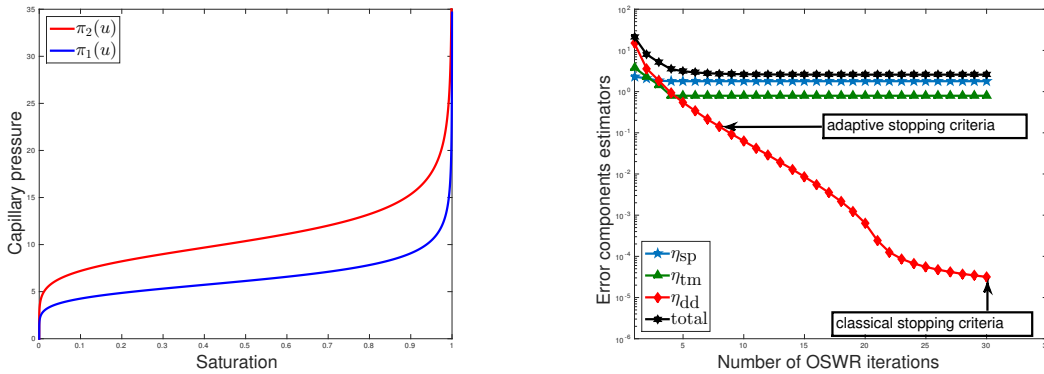


Figure 16: Test case 3: capillary pressure functions (left) and evolution of the spatial, temporal, and domain decomposition estimators as a function of the number of Robin-OSWR iterations (right)

The initial saturation is set equal to 0.05 in rock 1 while in rock 2, it is set so as to satisfy the equality of capillary pressure on the interface. We use Robin-OSWR method for this test case. The saturation and the capillary pressure are shown at the final time in Fig. 17, and one can see that the saturation is discontinuous across the interface, but that the capillary pressure is continuous. One can also see that because of the contrast in the capillary pressure field, the saturation front moves faster inside rock 2, allowing for a discontinuous change in saturation at the interface.

In Fig. 16 (right), we plot the different estimators as functions of the OSWR iterations when using the stopping criteria (8.2) with  $\delta_{dd} = 0.1$  and (8.1) with  $\delta_{lin} = 0.1$ . The non-adaptive OSWR needs 30 iterations to satisfy (9.3), while the adaptive OSWR only needs 8 iterations. Regarding the efficiency of the adaptive linearization stopping criterion (8.1), we observed that more than 2/3 of the Newton iterations needed to reach the classical linearization stopping criterion (9.3) can be saved.

Finally, in Fig. 18, the global error as well as the domain decomposition error are shown shown at the final time step. Again, as expected, the DD error does not affect the global error. Particularly, the error follows the saturation front which is discontinuous across the interface. Also, some space error on both sides of the interface and near the injection boundary can still be detected.

## 10 Conclusion

We proposed an adaptive domain decomposition algorithm that is global-in-time and works as follows:

1. At each DD iteration, the problem is solved independently in each subdomain on the whole time interval, and then Robin or Ventcell boundary data are exchanged across the space-time interface.

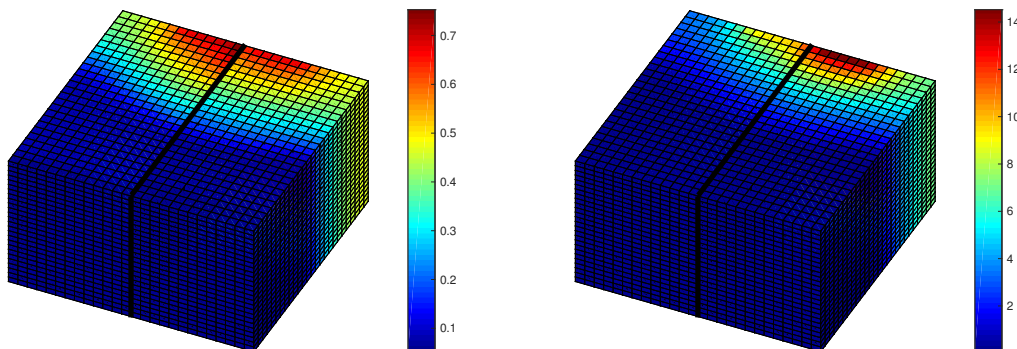


Figure 17: Test case 3: saturation (left) and capillary pressure (right) at final time

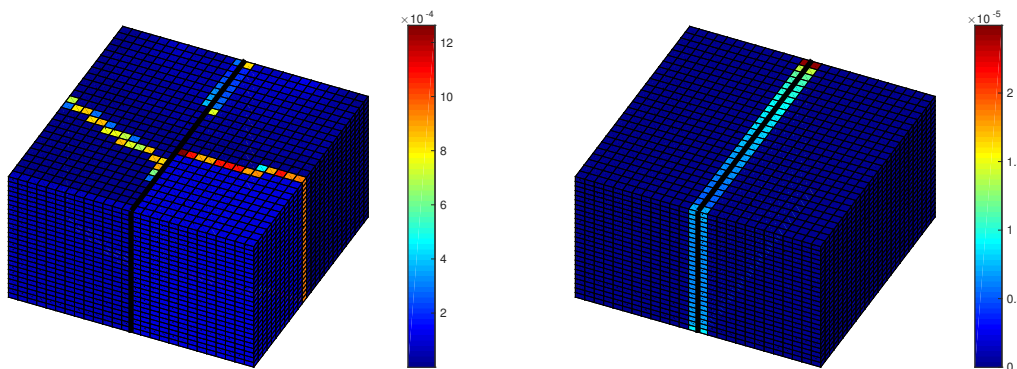


Figure 18: Test case 3: estimated error (left) and domain decomposition error (right) at final time

2. During the DD iteration and at each time and linearization steps, several estimators are computed. Then, the error induced by domain decomposition can be compared to that coming from linearization and spatial and temporal discretizations. The iterations are stopped when the DD estimator becomes smaller (up to a user-chosen constant) than the other error components.

The results confirm that this approach is applicable to the present degenerate parabolic problem with nonlinear and discontinuous transmission conditions. In particular, the DD estimator is a practical tool to estimate the DD error component, and combining optimized parameters and adaptive stopping criteria results in efficient OSWR algorithms. As a benefit, moreover, the overall error is guaranteed to lie below the computed overall estimate.

## Acknowledgments

This work is the result of a collaboration that took place during the CEMRACS summer school & projects 2016. We warmly thank the organizers as well as the CIRM for its welcome.

## A Details on the equilibrated flux reconstruction

We provide here the details on the reconstruction of an equilibrated flux satisfying (5.3), following closely [4, 5]. For each subdomain  $\Omega_i$ , we consider a subset  $B_i$  of  $\Omega_i$ , termed a band, which contains all the elements of  $\mathcal{T}_{h,i}$  that share a face, and edge, on a point with the interface  $\Gamma$ . We denote by  $\mathcal{T}_{h,i}^B$  the corresponding

submesh. We start from  $\mathbf{u}_{h,i}^{k,n,m}$  given by (5.4), which is subdomain-wise  $\mathbf{H}(\text{div})$ -conforming (belongs to  $\mathbf{RTN}_0(\Omega_i)$ ),  $i = 1, 2$  and set

$$\boldsymbol{\sigma}_h^{k,n,m}|_K := \mathbf{u}_h^{k,n,m}|_K, \quad \forall K \in \mathcal{T}_{h,i} \text{ s.t. } K \notin \mathcal{T}_{h,i}^B. \quad (\text{A.1})$$

In the bands, we will modify  $\mathbf{u}_h^{k,n,m}$  so as to arrive at (5.3); note that simply prescribing the normal components of  $\boldsymbol{\sigma}_h^{k,n,m}$  by  $\{\{\mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_{B_i}\}\}$  at the interface would lead to (5.3a) but not to (5.3b). We denote by  $\Gamma_i^b$  the boundaries (in 3D for the situation of Fig. 19,  $b = 1, 2, 3, 4$ ) of  $\partial B_i$  that intersect  $\partial\Omega$ , for  $i = 1, 2$ . We denote also by  $\Gamma_i^{\text{int}}$  the boundary of  $\partial B_i$  that is inside  $\Omega_i$ ,  $i = 1, 2$ , see Fig. 19. We then identify nine

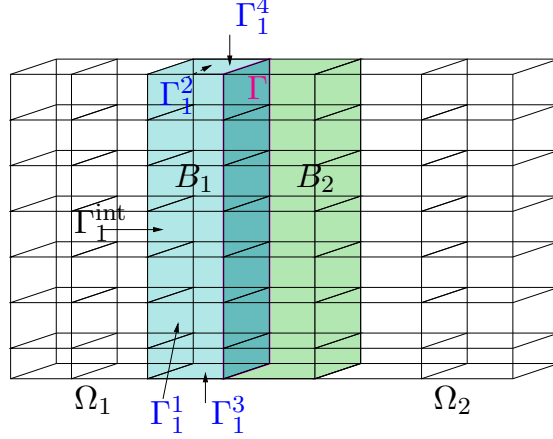


Figure 19: Bands  $B_1$  and  $B_2$  surrounding the interface  $\Gamma$  in three space dimensions

corrections  $(c_{\Gamma_1^b}^{k,n,m})_{1 \leq b \leq 4}$ ,  $(c_{\Gamma_2^b}^{k,n,m})_{1 \leq b \leq 4}$ , and  $c_{\Gamma}^{k,n,m}$  to the averaged flux  $\{\{\mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_{B_i}\}\}$  that will lead to equilibrium in each band  $B_i$ ,  $i = 1, 2$ . In other words, we seek to satisfy the two balancing conditions, for  $i = 1, 2$ :

$$\sum_{b=1}^4 c_{\Gamma_i^b}^{k,n,m} + (\mathbf{n}_{\Gamma} \cdot \mathbf{n}_{B_i}) c_{\Gamma}^{k,n,m} = \left( f_i^n - \frac{u_K^{k,n,m} - u_K^{k,n-1}}{\tau^n}, 1 \right)_{B_i} - (\{\{\mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_{B_i}\}\}, 1)_{\partial B_i}, \quad (\text{A.2})$$

Here  $\mathbf{n}_{\Gamma}$  is a unit vector normal to  $\Gamma$ , pointing either from  $\Omega_1$  to  $\Omega_2$ , or from  $\Omega_2$  to  $\Omega_1$ , and  $\mathbf{n}_{B_i}$  is the outward unit vector normal to  $\partial B_i$ .

The *coarse interface problem* (A.2) is solved via the *least squares minimization*, see [5] for the details. Finally, the corrections are distributed from the boundary of the bands to their interiors by approximating, using the mixed finite element or the finite volume method, the following local Neumann problems: find  $(q_{h,i}^{k,n,m}, \boldsymbol{\sigma}_{h,i}^{k,n,m}) \in \mathbb{P}_0(\mathcal{T}_{h,i}^B) \times \mathbf{RTN}_0(B_i)$  with  $(q_{h,i}^{k,n,m}, 1)_{B_i} = 0$  such that

$$\left\{ \begin{array}{ll} \nabla \cdot \boldsymbol{\sigma}_{h,B_i}^{k,n,m}|_K = f_i^n|_K - \frac{u_K^{k,n,m} - u_K^{k,n-1}}{\tau^n} & \forall K \in \mathcal{T}_{h,i}^B, \\ \boldsymbol{\sigma}_{h,B_i}^{k,n,m} - \mathbf{u}_{h,i}^{k,n,m} = -\nabla q_{h,i}^{k,n,m}, & \text{in appropriate weak sense in } B_i, \\ \boldsymbol{\sigma}_{h,B_i}^{k,n,m} \cdot \mathbf{n}_{\Gamma} = \mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_{\Gamma}, & \text{on } \Gamma_i^{\text{int}}, \\ \boldsymbol{\sigma}_{h,B_i}^{k,n,m} \cdot \mathbf{n}_{\Gamma} = \{\{\mathbf{u}_h^{k,n,m} \cdot \mathbf{n}_{\Gamma}\}\} + \frac{1}{|\Gamma|} c_{\Gamma}^{k,n,m}, & \text{on } \Gamma, \\ \boldsymbol{\sigma}_{h,B_i}^{k,n,m} \cdot \mathbf{n}_{\Gamma} = \mathbf{u}_{h,i}^{k,n,m} \cdot \mathbf{n}_{\Gamma} + \frac{1}{|\Gamma_i^b|} c_{\Gamma_i^b}^{k,n,m}, & \text{on } \Gamma_i^b. \end{array} \right.$$

We finally complement (A.1) by setting  $\boldsymbol{\sigma}_h^{k,n,m}|_{B_i} := \boldsymbol{\sigma}_{h,B_i}^{k,n,m}$ .

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