A posteriori error estimates and stopping criteria in a space-time domain decomposition method for two-phase flow with discontinuous capillary pressure

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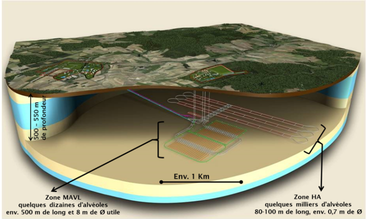
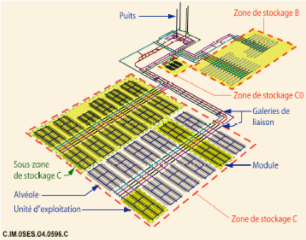
Outline

1. Motivations – physical problem
2. Domain decomposition
   - Optimized Schwarz Waveform Relaxation algorithm
   - Discretization – numerical example
3. A posteriori error estimates
   - Saturation and flux reconstruction
   - A posteriori stopping criteria
   - Numerical examples

Geological repository for nuclear waste

Deep underground repository
(High-level waste)





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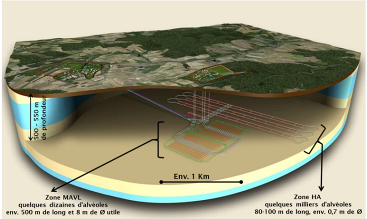

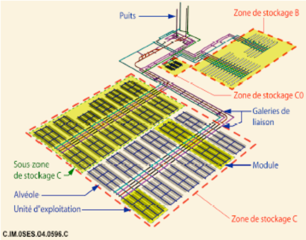

Challenges

- Different materials $\rightarrow$ strong heterogeneity, different time scales.
- Large differences in spatial scales.
- Long-term computations.

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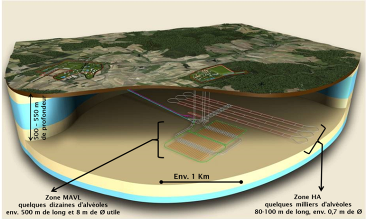

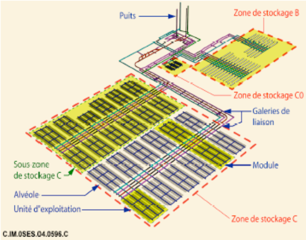

Challenges

- Different materials $\rightarrow$ strong heterogeneity, different time scales.
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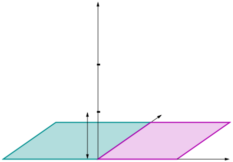
- Use space-time DD
- Estimate the error at DD iterations
- Develop criteria to stop DD iterations as soon as the discretization error is reached

Space–time domain decomposition

Domain decomposition in space



- Discretize in time and apply the DD algorithm at each time step:

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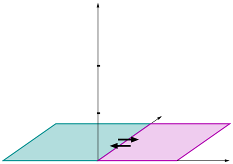

- Discretize in time and apply the DD algorithm at each time step:
  - Solve stationary problems in the subdomains
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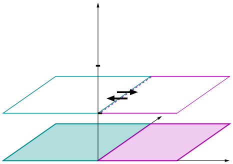

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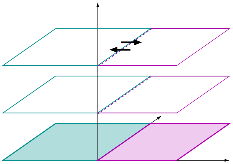

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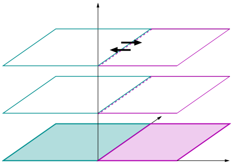

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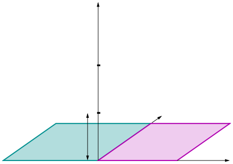

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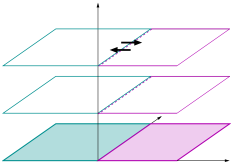

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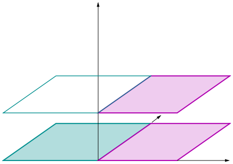

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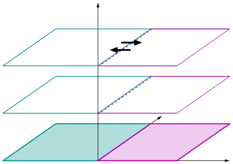

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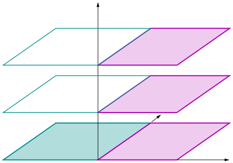

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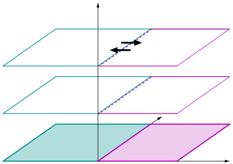

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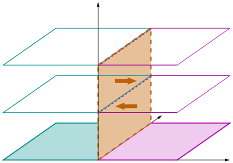

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- Exchange information through the space-time interface [Halpern-Nataf-Gander (03), Martin (05)]

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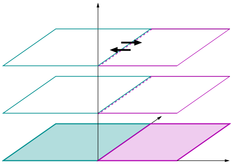

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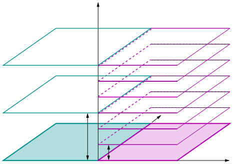
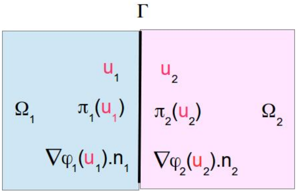


- Solve time-dependent problems in the subdomains
- Exchange information through the space-time interface [Halpern-Nataf-Gander (03), Martin (05)]

✓ Different time steps can be used in each subdomain according to its physical properties. [Halpern–Japhet–Szeftel (12), Hoang–Japhet–Jaffré–M.K.–Roberts (13)]

Physical problem: two–phase flow with 2 rock types

Two–phase (water – gas) immiscible flow, neglect advection (capillary trapping)
(Enchery, Eymard, Michel (06), Cances (08))
$u \in [0, 1]$: gas saturation. $\pi(u)$ capillary pressure, increasing on $[0, 1]$, $\varphi(u)$: Kirchhoff transform



Nonlinear diffusion equation

$\partial_t u - \Delta\varphi(u) = 0 \quad$ in $\Omega \times [0, T]$

$\varphi(u) = \varphi(g)$ on $\partial\Omega \times [0, T]$, $\quad u(., 0) = u_0(.)$ in Ω

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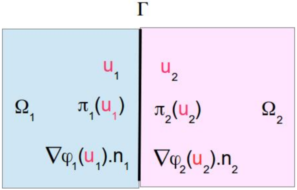

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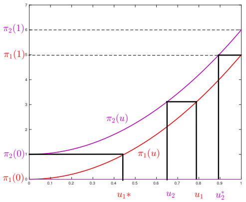
Physical transmission conditions: continuity of

Cap. pressure Need to *truncate* cap. pressure functions
[Chavent, Jaffré (86)], [Ern, Mozolewski, Schuh (10)]

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

Fluxes $\nabla\varphi_1(u_1) \cdot \mathbf{n}_1 = -\nabla\varphi_2(u_2) \cdot \mathbf{n}_2$ on Γ



2 different nonlinearities. Both u and $\varphi(u)$ discontinuous across Γ.

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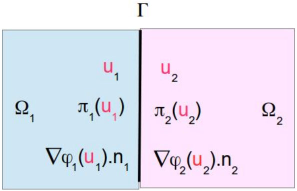

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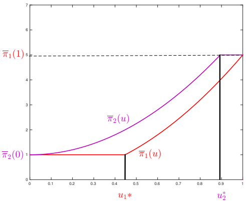

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Optimized Schwarz Waveform Relaxation algorithm (OSWR)

Equivalent space–time multidomain formulation

Solve the space-time coupled problem, with $i = 1, 2$:

$$\partial_t u_i - \Delta\varphi_i(u_i) = 0 \qquad \text{in } \Omega_i \times [0, T]$$

with physical transmission conditions on space–time interface $\Gamma \times [0, T]$

$$\begin{aligned} \bar{\pi}_1(u_1) &= \bar{\pi}_2(u_2) \\ \nabla\varphi_2(u_2)\cdot n_2 &= -\nabla\varphi_1(u_1)\cdot n_1 \end{aligned}$$

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with Robin transmission conditions on space–time interface $\Gamma \times [0, T]$

$$\nabla \varphi_1(u_1) \cdot n_1 + \alpha_{12} \bar{\pi}_1(u_1) = -\nabla \varphi_2(u_2) \cdot n_2 + \alpha_{12} \bar{\pi}_2(u_2)$$
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For $k \geq 0$, solve **in parallel** the **space-time** Robin subdomain problems ($i = 1, 2$):

$$\partial_t u_i^k - \Delta\varphi_i(u_i^k) = 0 \qquad \text{in } \Omega_i \times (0, T)$$
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- Start with $-\nabla\varphi_j(u_j^0)\cdot n_j + \alpha_{ij}(\bar{\pi}_j(u_j^0) = g_i^0$ a given function, $i = 1, 2$.
- Basic ingredient: subdomain solver with Robin BC (existence proof in progress)
- α_{ij} free coefficients, chosen to optimize convergence rate
  [Gander (06), Japhet, Nataf (01)], [Halpern, Hubert (14)], [Caetano, Gander, Halpern, Szeftel (10)]

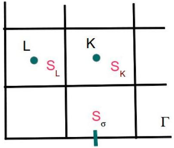
Discretization

In space: two-point finite volumes

Two-point finite volume scheme on rectangular mesh, additional unknowns at the centers of the faces on the interface

At each OSWR iteration k, at each time step n, solve non-linear system over each subdomain i for

$$u^k_{h,\tau} = \left\{ (u_K^{n+1,k})_{K\in\mathcal{T}_i}, (u_\sigma^{n+1,k})_{\sigma\in\mathcal{E}_{i,\Gamma}} \right\}$$



Implemented with Matlab Reservoir Simulation Toolbox ([Lie et al. (14)])

Solver with automatic differentiation : no explicit programming of Jacobian

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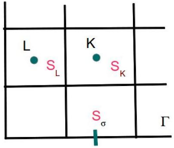

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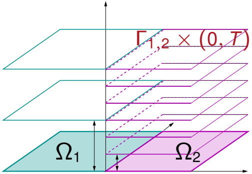
In time: DG0

Piecewise constant functions, identical to backward Euler, with numerical integration for source term.

Non conforming time grids: Information on one time grid at the interface is passed to the other time grid at the interface using L2-projections.

Use an optimal projection algorithm

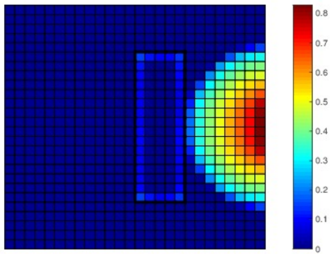
[Gander-Japhet-Maday-Nataf (05), Gander, Japhet (13)]



DNAPL infiltration: trapping by a low capillarity lens

Mobilities $\lambda_{o,i}(u) = u^2$, and $\lambda_{g,i}(u) = 3(1-u)^2$, $i \in \{1, 2\}$,

Capillary pressure $\pi_1(u) = \ln(1-u)$, and $\pi_2(u) = 0.5 - \ln(1-u)$.



Evolution of saturation ($t = 100, 200, 350, 480$)

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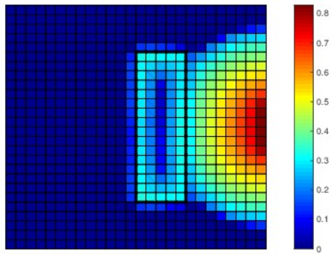

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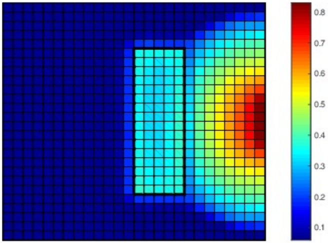

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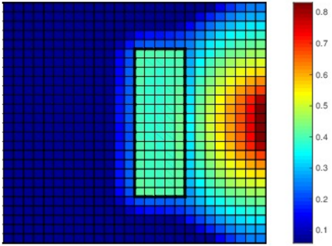

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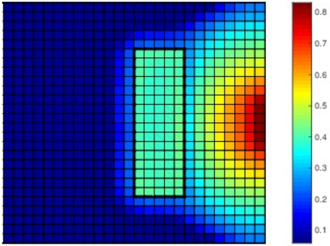

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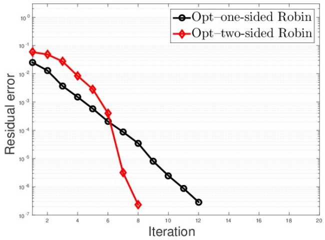

Convergence curve

A posteriori error estimates: overview

$$\underbrace{||u - \tilde{u}_{h\tau}^k||}_{\textbf{unknown}} \leq \underbrace{\eta_{\mathrm{SP}}^k + \eta_{\mathrm{TM}}^k + \eta_{\mathrm{DD}}^k}_{\text{Fully computable estimators}}$$

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- Error estimators depend on $H(\text{div}, \Omega)$ flux and $H^1(\Omega)$ potential reconstruction [Vohralík (10), Pencheva-Vohralík-Wheeler-Wildey (13), Di Pietro, Vohralík, Yousef (15)]
- Separate (time, space) discretization and DD estimators : enables stopping criteria for DD iterations [Rey, Rey, Gosselet (14), Ern, Vohralík (15)]
- Extension to finite volume, Robin BC (no conformity) [Ali Hassan, Japhet, M. K., Vohralík (18)]
- In finite volume, $u_{h\tau}^k$ piecewise constant, so $\nabla u_{h\tau}^k = 0$, cannot be used for energy estimates

A posteriori error estimates: overview

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Main steps

- Saturation and flux reconstructions
- Bound error measure by computable estimates

Saturation and flux reconstruction

Post-processing of $u^k_{h\tau}$

Each iteration k and at each time step, construct *locally* (per element)

- $\mathbf{q}^{n,k}_{h,i} \in \mathbf{RTN}_0(\Omega_i) \subset H(\mathrm{div}, \Omega_i)$ with fluxes matching that of $\varphi_i(u^{n,k}_K)$,
- Post–processed $\tilde{\varphi}^k_{h\tau,i} \in \mathbf{P}_2(\mathcal{T}_i)$, linear in time, and saturation $\tilde{u}^{n,k}_{h\tau} = \varphi_i^{-1}(\tilde{\varphi}^{k,n}_{hi})$

Non–linearity: need to construct both $\tilde{\varphi}^k_{h\tau,i}$ and $\tilde{u}^{n,k}_{h\tau}$ ($\tilde{u}^{n,k}_{h\tau}$ for theory only).

Saturation and flux reconstruction

Post-processing of $u_{h\tau}^k$

Each iteration k and at each time step, construct *locally* (per element)

- $\mathbf{q}_{h,i}^{n,k} \in \mathbf{RTN}_0(\Omega_i) \subset H(\text{div}, \Omega_i)$ with fluxes matching that of $\varphi_i(u_K^{n,k})$,
- Post–processed $\tilde{\varphi}_{h\tau,i}^k \in \mathbf{P}_2(\mathcal{T}_i)$, linear in time, and saturation $\tilde{u}_{h\tau}^{n,k} = \varphi_i^{-1}(\tilde{\varphi}_{hi}^{k,n})$

Non–linearity: need to construct both $\tilde{\varphi}_{h\tau,i}^k$ and $\tilde{u}_{h\tau}^{n,k}$ ($\tilde{u}_{h\tau}^{n,k}$ for theory only).

- ✗ FV method, so $\tilde{u}_{h\tau}^k \notin H^1(\Omega_i)$
- ✗ Robin DD method so $\tilde{u}_{h\tau}^k$ jumps across Γ and no continuous flux approximation

Saturation and flux reconstructions:

- $s_{h\tau}^k$: $H^1(\Omega)$-conforming, continuous and piecewise linear in time. Modify on Γ to ensure continuity of capillary pressure
- $\sigma_{h\tau}^k$: $H(\text{div}, \Omega)$-conforming and local conservative in each element, piecewise constant in time. Solve coarse problem to ensure continuous flux across Γ.

Saturation post–processing and reconstruction

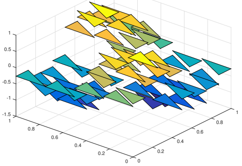

Figure: $u_{h\tau}^{k}$

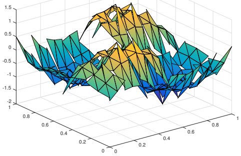

Figure: $\tilde{u}_{h\tau}^{k}$

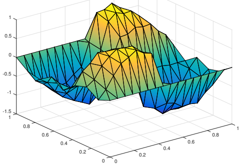

Figure: $s_{h\tau}^{k}$

Error estimators and error measures

Local estimators

Spatial disc. $\eta^{n,k}_{\mathrm{SP},K,i} := 1/\pi\, h_K \|\partial_t s^k_{h,\tau} + \nabla \cdot \sigma^{k,n}_h\|_K + \|\nabla \varphi_i(s^k_{h,\tau}(\cdot, t_n)) + \mathbf{q}^{k,n}_{h,i}\|_K,$

Time disc. $\eta^{n,k}_{\mathrm{TM},K,i}(t) := \|\nabla\big(\varphi_i(s^k_{h,\tau}(\cdot, t)) - \varphi_i(s^k_{h,\tau}(\cdot, t_n))\big)\|_K$

DD error $\eta^{n,k}_{\mathrm{DD},K,i} := \|\mathbf{q}^{n,k}_{h,i} - \sigma^{n,k}_h\|_K$

Global versions η^k_{SP}, η^k_{TM}, η^k_{DD} built by summation over the mesh, the timesteps and the subdomains.

Can be extended to include effect of linearization for subdomain problem. See [Di Pietro, Vohralík, Yousef (15)].

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Error measures for the approximate solution

Exact solution $u \in H^1(0,T;H^{-1}(\Omega))$, with $\varphi_i(u|_{\Omega_i}) \in L^2(0,T;H^1(\Omega_i))$, $(i=1,2)$.

Strong distance $\|u - \tilde{u}^k_{h,\tau}\|_\sharp$, linked to energy norm

Weak distance $\|u - s^k_{h,\tau}\|_\flat$, linked to dual norm of the residual

Actually defined for any function in the above spaces.

A posteriori error estimate

Let L_{φ_i} Lipschitz constant of φ_i, $L_\varphi := \max(L_{\varphi_1}, L_{\varphi_2})$,
Initial condition estimator: $\eta_{\mathrm{IC}}^k := \|u_0 - s_{h,\tau}^k(\cdot, 0)\|_{H^{-1}(\Omega)}$,

Theorem

- *Error bounds in "weak distance"*

$$\|u - s_{h,\tau}^k\|_\flat \leq \sqrt{L_\varphi/2}\sqrt{2e^T - 1}\eta_{\mathrm{IC}}^k + \eta_{\mathrm{SP}}^k + \eta_{\mathrm{TM}}^k + \eta_{\mathrm{DD}}^k,$$

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- *Error bound in "strong distance"*
  Assume $\bar{\varphi} \in L^2(0, T, H_0^1(\Omega))$, *with* $\bar{\varphi}|_{\Omega_i} := \varphi_i(u_i) - \varphi_i(s_{h,\tau_i}^k), \quad i = 1, 2.$ *Then*

$$\|u - \tilde{u}_{h,\tau}^k\|_\sharp \leq \sqrt{L_\varphi/2}\sqrt{2e^T - 1}\eta_{\mathrm{IC}}^k + \eta_{\mathrm{SP}}^k + \eta_{\mathrm{TM}}^k + \eta_{\mathrm{DD}}^k + \|\tilde{u}_{h,\tau}^k - s_{h,\tau}^k\|_\sharp$$

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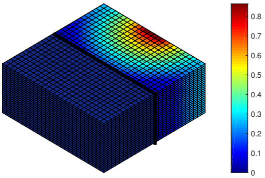
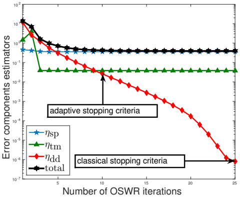
Remark

- Proof follows from [Di Pietro, Vohralík, Yousef (15)]
- Assumption above means capillary pressure must be continuous.

Two rock-types, flow across the interface

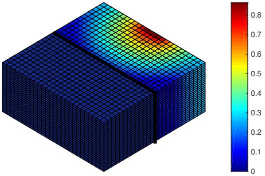


Subdomain decomposition and snapshot of saturation

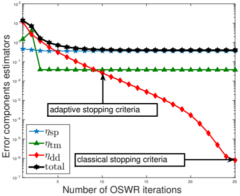


Evolution of the spatial, temporal, and DD estimators vs number of Robin OSWR iterations

Two rock-types, flow across the interface



Subdomain decomposition and snapshot of saturation



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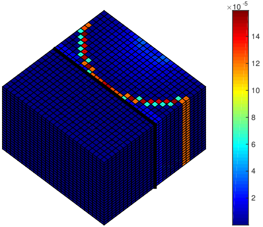
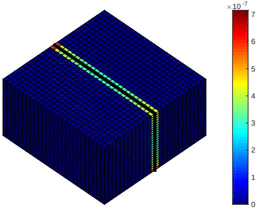


Global error



DD error

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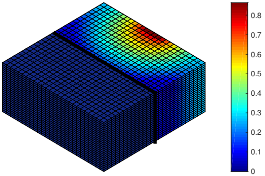

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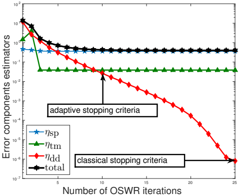

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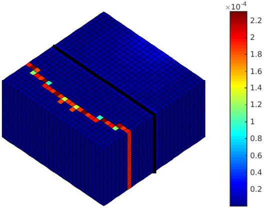

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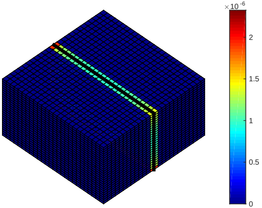
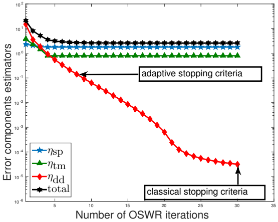
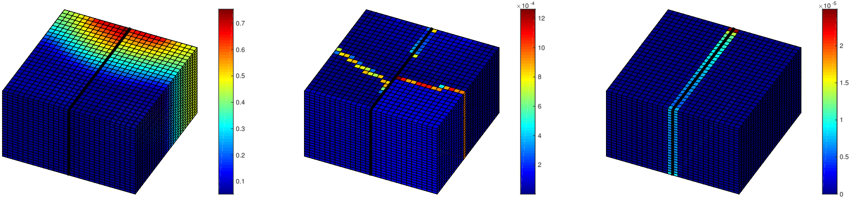


DD error

Two rock-types, flow along the interface

Capillary pressure and mobilities given by van Genuchten model $\pi_i(u) = P_i\left((1-u)^{-1/m} - 1\right)^{1/n}$, Parameters $n = 2.8$, $m = 1 - 1/n$, $P_1 = 10$, $P_2 = 5$.





Saturation (left), total error estimator (center) and DD error estimator (right)

Some references

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Comp. Meth. Appl. Math., vol. 18 (3), pp. 495–520, 2018

E. Ahmed, C. Japhet, M. K.
A Finite Volume Schwarz Algorithm for Two-Phase Immiscible Flow with Different Rock Types
In preparation

E. Ahmed, S. Ali Hassan, C. Japhet, M. K., M. Vohralík
A posteriori error estimates and stopping criteria for space-time domain decomposition for two-phase flow between different rock types
SMAI J. Comp. Math., in review

Post-processing $\tilde{u}^k_{h\tau,i}$ of $u^k_{h\tau,i}$

Each iteration k and at each time step

1. Construct $\mathbf{q}^{n,k}_{h,i} \in \mathbf{RTN}_0(\Omega_i) \subset H(\mathrm{div}, \Omega_i)$ such that

$$(\mathbf{q}^{n,k}_{h,i} \cdot \mathbf{n}_i, 1)_\sigma = \tau_\sigma(\varphi_i(u^{n,k}_K) - \varphi_i(u^{n,k}_L)), \quad \forall K \in \mathcal{T}_i, \forall L \in \mathcal{N}(K)$$

2. Construct locally $\tilde{\varphi}^k_{h\tau,i} \in \mathbf{P}_2(\mathcal{T}_i)$ by

$$-\nabla \tilde{\varphi}^{k,n}_{h,i}|_K = \mathbf{q}^{k,n}_{h,i}|_K, \quad \forall K \in \mathcal{T}_{h,i},$$

$$\frac{(\tilde{\varphi}^{k,n}_{h,i}, 1)_K}{|K|} = \varphi(u^{k,n}_K), \quad \forall K \in \mathcal{T}_{h,i}.$$

3. Define the post-processed saturation, piecewise linear in time, by (for theory only)

$$\tilde{u}^{k,n,}_{h,i} := \varphi_i^{-1}(\tilde{\varphi}^{k,n}_{hi}).$$

✖ $\tilde{u}^{k,n,}_{h,i} \notin H^1(\Omega_i)$ (same for $\tilde{\varphi}^{n,k}_{h,i}$).

Reconstruction of a conforming saturation

1. Construct piecewise polynomial $\hat{\varphi}_{h,i}^{n,k}$ by

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

   where $\mathcal{I}_{\text{av}}(p)(\mathbf{a}) = \frac{1}{|\mathcal{T}_{\mathbf{a}}|} \sum_{K \in \mathcal{T}_{\mathbf{a}}} p|_K(\mathbf{a})$.
   Cannot work directly with $\tilde{u}_{h,i}^{k,n,}$, as it is not a polynomial.

2. Define $s_{h,i}^{n,k} \in H^1(\Omega_i)$ by $s_{h,i}^{n,k} = \varphi^{-1}(\hat{\varphi}_{h,i}^{n,k})$ at the Lagrange DOFs.

3. Modify $s_{h,i}^{n,k}$ to satisfy
   - $\bar{\pi}_1(s_{h,1}^{n,k}) = \bar{\pi}_2(s_{h,2}^{n,k})$ at all nodes on Γ,
   - $\dfrac{1}{|K|}(s_{h,i}^{n,k}, 1) = u_K^{n,k}, \quad \forall K \in \mathcal{T}_i$ (use a bubble function)

Equilibrated flux reconstruction $\sigma_{h\tau}^k$

Build $\sigma_{h\tau}^k \in P_\tau^0(H(\mathrm{div},\Omega))$ such that

$$(\mathrm{div}\sigma_h^{n,k}, 1)_K = (-\frac{u_K^{n+1,k} - u_k^{n,k}}{\Delta t}, 1)_K, \qquad \forall K \in \mathcal{T}.$$

1. Set $\sigma_{h,i}^{n,k} = \mathbf{q}_{h,i}^{n,k} \in H(\mathrm{div},\Omega_i)$.
2. Compute "mass balance misfit" across Γ

$$\mathbf{r}_K = (\frac{u_K^{n+1,k} - u_k^{n,k}}{\Delta t}, 1)_{\Omega_i} + \langle \{\!\{\mathbf{q}_K^{n,k} \cdot \boldsymbol{n}_{\partial\Omega_i}\}\!\}, 1\rangle_{\partial\Omega_i}, \forall K \in \mathcal{T}$$

3. Solve a coarse least squares problem to redistribute $\mathbf{r}$ to boundaries of bands across interface
4. Solve local (well posed) Neumann problems in each band to recreate mass balance