A posteriori error estimates, stopping criteria, and adaptivity for multiphase compositional Darcy flows in porous media

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Outline

In a nutshell I

- In the context of petroleum reservoir engineering, numerical simulation is used to predict oil production and to plan exploitation
- Modelling the flow of several fluids through a porous medium leads to highly nonlinear and computationally expensive problems
- **Goal** significantly reduce simulation time
- **Idea** use a posteriori error estimators to make smart online choices

In a nutshell II

Fix $\mathcal{M}^0$ and τ_0. Set $t^0 \leftarrow 0$, $n \leftarrow 0$ and set the initial solution $\mathcal{X}_{h\tau}^0$.
while $t^n \leq t^F$ **do**
  Set $n \leftarrow n+1$, $\mathcal{M}^n \leftarrow \mathcal{M}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$.
  repeat { Equilibration of spatial and temporal errors }
    Set $k \leftarrow 0$ and $\mathcal{X}_{h\tau}^{n,0} \leftarrow \mathcal{X}_{h\tau}^{n-1}$.
    repeat { Newton iterations }
      $k \leftarrow k+1$ and $i \leftarrow 0$. Set $\mathcal{X}_{h\tau}^{n,k,0} := \mathcal{X}_{h\tau}^{n,k-1}$.
      Set up the linear system
      repeat { Algebraic iterations }
        Set $i = i+1$ and perform one iteration of the algebraic solver
        Compute $\eta_{\mathrm{sp}}^{n,k,i}$, $\eta_{\mathrm{tm}}^{n,k,i}$, $\eta_{\mathrm{lin}}^{n,k,i}$, $\eta_{\mathrm{alg}}^{n,k,i}$
      until stopping criterion
    until stopping criterion
    Adapt the time step τ^n
  until time-space equilibration
  Set $\mathcal{X}_{h\tau}^n \leftarrow \mathcal{X}_{h\tau}^{n,k,i}$, and $t^n \leftarrow t^{n-1} + \tau^n$.
end while

In a nutshell III

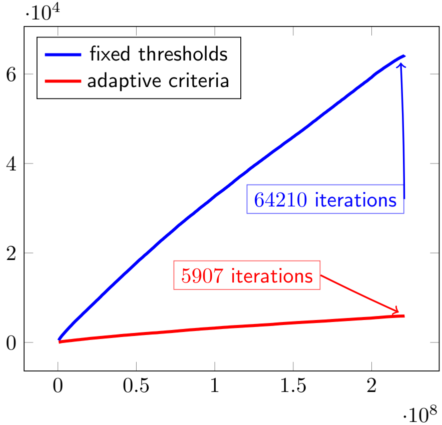

Figure: Cumulated linear solver iteration as a function of stopping criteria

The compositional Darcy model I

- Let two sets of phases $\mathcal{P}$ and components $\mathcal{C}$ be given
- We define for all $p \in \mathcal{P}$ and all $c \in \mathcal{C}$ the relevant subsets

$$\mathcal{C}_p := \{c \in \mathcal{C};\ c \text{ is present in } p\}\,, \quad \mathcal{P}_c := \{p \in \mathcal{P};\ c \text{ is present in } p\}$$

	H_2O	CO_2	N_2	C_7H_{16}
w	✓	✗	✗	✗
h	✗	✓	✓	✓
o	✗	✓	✓	✓

Figure: Example of a two-phase, three-component flux

The compositional Darcy model II

- Formulation inspired by [Coats, 1980, Eymard et al., 2012]
- The unknowns of the model are

$$\mathcal{X} := \begin{pmatrix} P \\ (S_p)_{p\in\mathcal{P}} \\ (C_{p,c})_{p\in\mathcal{P},c\in\mathcal{C}_p} \end{pmatrix} = \begin{pmatrix} P \\ \boldsymbol{S} \\ (\boldsymbol{C}_p)_{p\in P} \end{pmatrix}$$

- We define for all $p \in \mathcal{P}$ the phase pressure as

$$P_p(P, \boldsymbol{S}) = P + P_{\mathrm{c}_p}(\boldsymbol{S})$$

- The (average) phase velocity is given by Darcy's law

$$\boldsymbol{v}_p = -\boldsymbol{\Lambda}\left(\nabla P_p + \rho_p g \nabla z\right)$$

The compositional Darcy model III

- Let Ω denote the space domain and $t_\mathrm{F} > 0$ the simulation time
- Conservation of the quantity of matter: For all $c \in \mathcal{C}$,

$$\boxed{\partial_t l_c + \nabla\cdot\mathbf{\Phi}_c = q_c \quad \text{in } \Omega \times (0, t_\mathrm{F})}$$

with q_c source piecewise constant in space-time and

$$l_c := \phi \sum_{p\in\mathcal{P}_c} \zeta_p S_p C_{p,c}, \qquad \mathbf{\Phi}_c := \sum_{p\in\mathcal{P}_c} \left\{\mathbf{\Phi}_{p,c} := \nu_p C_{p,c} \boldsymbol{v}_p\right\},$$

- Initial and boundary conditions

$$l_c(0) = l_c^0 \text{ in } \Omega, \quad \mathbf{\Phi}_c\cdot\boldsymbol{n}_\Omega = 0 \text{ on } \partial\Omega \times (0, t_\mathrm{F})$$

The compositional Darcy model IV

- Saturation of the pore volume

$$\sum_{p\in\mathcal{P}} S_p = 1$$

- Partition of the matter into components

$$\sum_{c\in\mathcal{C}_p} C_{p,c} = 1 \quad \forall p \in \mathcal{P}$$

- Thermodynamic equilibrium relations close the system

A classical finite volume scheme I

- We consider a popular fully implicity finite volume discretization
- The numerical fluxes are based on phase-upwind and two-point fluxes
- On phase-upwind cf., e.g., [Brenier and Jaffré, 1991]

A classical finite volume scheme II

- We consider a partition $(t^n)_{0\leq n\leq N}$ of $(0,t_{\mathrm{F}})$ with

$$t^n = \sum_{i=1}^{n} \tau_i \qquad \tau_i > 0 \quad \forall 1 \leq i \leq n$$

- We denote by $(\mathcal{M}^n)_{0\leq n\leq N}$ a sequence of meshes of Ω with

$$\mathcal{M}^n = \{M\}$$

- The discrete unknowns are, for all $M \in \mathcal{M}^n$,

$$\mathcal{X}^n_{\mathcal{M}} := (\mathcal{X}^n_M)_{M\in\mathcal{M}^n}, \quad \mathcal{X}^n_M := \begin{pmatrix} P^n_M \\ \boldsymbol{S}^n_M \\ (\boldsymbol{C}^n_{p,M})_{p\in\mathcal{P}} \end{pmatrix}$$

A classical finite volume scheme III

- For each phase, the discrete phase pressure is given by

$$P_{p,M}^n(P_M^n, \boldsymbol{S}_M^n) = P_M^n + P_{c_p}(\boldsymbol{S}_M^n) \quad \forall M \in \mathcal{M}^n$$

- The discrete phase velocity is given by, for all $\sigma \subset \partial M \cap \partial L$,

$$F_{p,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) := |\sigma| \frac{\alpha_M \alpha_L}{\alpha_M + \alpha_L} \left[P_{p,M}^n - P_{p,L}^n + \rho_{p,\sigma}^n g \left(z_M - z_L\right)\right],$$

while $F_{p,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) = 0$ if $\sigma \subset \partial\Omega$

A classical finite volume scheme IV

- Discrete conservation of the quantity of matter: For all $c \in \mathcal{C}$,

$$\boxed{|M|\partial_t^n l_{c,M} + \sum_{\sigma \in \mathcal{E}_M^{\mathrm{i},n}} F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) = |M| q_{c,M}^n \quad \forall M \in \mathcal{M}^n}$$

with

$$l_{c,M}^n = \phi \sum_{p \in \mathcal{P}_c} \zeta_p(P_{p,M}^n, \boldsymbol{C}_{p,M}^n) S_{p,M}^n C_{p,c,M}^n$$

and molar component flux

$$F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) := \sum_{p \in \mathcal{P}_c} \left\{ F_{p,c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) := \nu_p^{\uparrow} C_{p,c,M_p^{\uparrow}}^n F_{p,M,\sigma}(\mathcal{X}_{\mathcal{M}}^n) \right\}$$

- Closure laws are enforced cell-wise

Outline

Essential bibliography

- A posteriori estimates for model unsteady nonlinear problems
  - [Eriksson and Johnson, 1995, Verfürth, 1998a, Verfürth, 1998b]
- A posteriori estimates for degenerate parabolic problems
  - [Nochetto et al., 2000, Ohlberger, 2001]
  - [Di Pietro et al., 2013b, Di Pietro et al., 2013a]
- Adaptive mesh refinement in reservoir simulation
  - [Heinemann, 1983, Ewing et al., 1989] and many more
  - [Mamaghani et al., 2011] (SAGD with $\#\mathcal{C} = 2$, $\#\mathcal{P} = 3$)
- Smart online choices
  - [Jiránek et al., 2010] (stopping criteria)
  - [Ern and Vohralík, 2013] (inexact Newton)
  - [Di Pietro et al., 2013b] (stopping criteria + parameter selection)

Fully computable upper bound I

Assumption (Weak solution)

There exists a weak solution $\mathcal{X}$ such that

- *For all $p \in \mathcal{P}$, $P_p(P, \boldsymbol{S}) \in X := L^2(H^1(\Omega))$*
- *For all $c \in \mathcal{C}$, $l_c \in Y := H^1(L^2(\Omega))$ and $\boldsymbol{\Phi}_c \in [L^2(L^2(\Omega))]^d$*
- *The following equality holds for all $\varphi \in X$ and all $c \in \mathcal{C}$:*

$$\int_0^{t_\mathrm{F}} \{(\partial_t l_c, \varphi)(t) - (\boldsymbol{\Phi}_c, \nabla\varphi)(t)\} \,\mathrm{d}t = \int_0^{t_\mathrm{F}} (q_c, \varphi)(t)\mathrm{d}t$$

- *The initial condition and the closure equations hold*

We equip the space X with the norm

$$\|\varphi\|_X := \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{M \in \mathcal{M}^n} \|\varphi\|_{X,M}^2 \mathrm{d}t \right\}^{1/2}, \quad \|\varphi\|_{X,M}^2 := \varepsilon h_M^{-2} \|\varphi\|_M^2 + \|\nabla\varphi\|_M^2$$

Fully computable upper bound II

$$\mathcal{N} := \left\{ \sum_{c\in\mathcal{C}} \mathcal{N}_c^{\,2} \right\}^{1/2} + \left\{ \sum_{p\in\mathcal{P}} \mathcal{N}_p^{\,2} \right\}^{1/2}$$

- Dual norm of the residual

$$\mathcal{N}_c := \sup_{\varphi\in X, \|\varphi\|_X=1} \int_0^{t_{\mathrm{F}}} \left\{ (\partial_t l_c - \partial_t l_{c,h\tau}, \varphi)(t) - \left(\boldsymbol{\Phi}_c - \boldsymbol{\Phi}_{c,h\tau}, \nabla\varphi \right)(t) \right\} \mathrm{d}t$$

with $\boldsymbol{\Phi}_{c,h\tau} = \sum_{p\in\mathcal{P}_c} \nu_p(P_{p,h\tau}, \boldsymbol{S}_{h,\tau}, \boldsymbol{C}_{p,h\tau}) C_{p,c,h\tau} \boldsymbol{v}_p(P_{p,h\tau}, \boldsymbol{C}_{p,h\tau})$

- Nonconformity in X:

$$\mathcal{N}_p := \inf_{\varphi_p\in X} \left\{ \sum_{c\in\mathcal{C}_p} \int_0^{t_{\mathrm{F}}} \|\boldsymbol{\Psi}_{p,c}(P_{p,h\tau})(t) - \boldsymbol{\Psi}_{p,c}(\varphi_p)(t)\|^2 \mathrm{d}t \right\}^{1/2}$$

with $\boldsymbol{\Psi}_{p,c}(\varphi) := \nu_p(P_{p,h\tau}, \boldsymbol{S}_{h\tau}, \boldsymbol{C}_{p,h\tau}) C_{p,c,h\tau} \boldsymbol{\Lambda} \nabla\varphi$

Fully computable upper bound III

Theorem (Fully computable upper bound)

The following guaranteed upper bounds hold:

$$\mathcal{N}_c \leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta^n_{\mathrm{R},M,c} + \eta^n_{\mathrm{F},M,c}(t)\right)^2 \mathrm{d}t \right\}^{1/2} \quad \forall c \in \mathcal{C},$$

$$\mathcal{N}_p \leq \left\{ \sum_{c\in\mathcal{C}_p} \sum_{n=1}^{N} \int_{I_n} \sum_{M\in\mathcal{M}^n} \left(\eta^n_{\mathrm{NC},M,p,c}(t)\right)^2 \mathrm{d}t \right\}^{1/2} \quad \forall p \in \mathcal{P},$$

with estimators given by, for all $c \in \mathcal{C}$ and all $M \in \mathcal{M}^n$,

$$\begin{aligned}
\eta^n_{\mathrm{R},M,c} &:= \tilde{C}_{\mathrm{P},M} h_M \|q^n_{c,h} - \partial^n_t l_{c,h\tau} - \nabla\cdot\boldsymbol{\Theta}^n_{c,h}\|_M,\\
\eta^n_{\mathrm{F},M,c}(t) &:= \|\boldsymbol{\Theta}^n_{c,h} - \boldsymbol{\Phi}_{c,h\tau}(t)\|_M,\\
\eta^n_{\mathrm{NC},M,p,c}(t) &:= \|\boldsymbol{\Psi}_{p,c}(P_{p,h\tau})(t) - \boldsymbol{\Psi}_{p,c}(\mathfrak{P}_{p,h\tau})(t)\|_M \quad \forall p \in \mathcal{P}_c.
\end{aligned}$$

where, for all $c \in \mathcal{C}$, $\boldsymbol{\Theta}^n_{c,h} \in \mathbf{RTN}(\mathcal{M}^n)$ s.t.

$$\boxed{(q^n_{c,h} - \partial^n_t l_{c,h\tau} - \nabla\cdot\boldsymbol{\Theta}^n_{c,h}, 1)_M = 0 \quad \forall M \in \mathcal{M}^n.}$$

Linearization and algebraic resolution I

- Solving the discrete problem amounts to zeroing the residuals

$$R_{c,M}^n(\mathcal{X}_\mathcal{M}^n) := |M|\frac{l_{c,M}(\mathcal{X}_M^n) - l_{c,M}^{n-1}}{\tau^n} + \sum_{\sigma\in\mathcal{E}_M^{\mathrm{i},n}} F_{c,M,\sigma}(\mathcal{X}_\mathcal{M}^n) - |M| q_{c,M}^n = 0$$

- The Newton method generates a sequence $(\mathcal{X}_\mathcal{M}^{n,k})_{k\geq 0}$ by solving

$$\sum_{M'\in\mathcal{M}^n} \frac{\partial R_{c,M}^n}{\partial \mathcal{X}_{M'}^n}(\mathcal{X}_\mathcal{M}^{n,k-1}) \cdot (\mathcal{X}_{M'}^{n,k} - \mathcal{X}_{M'}^{n,k-1}) + R_{c,M}^n(\mathcal{X}_\mathcal{M}^{n,k-1}) = 0$$

Linearization and algebraic resolution II

- The resulting linear system can be solved by an iterative linear solver
- The residuals at Newton iteration k and linear solver iteration i read

$$R_{c,M}^{n,k,i} = |M| \frac{l_{c,M}\left(\mathcal{X}_{\mathcal{M}}^{n,k-1}\right) + \mathcal{L}_{c,M}^{n,k,i} - l_{c,M}^{n-1}}{\tau^n} + \sum_{\sigma \in \mathcal{E}_M^{\mathrm{i},n}} F_{c,M,\sigma}^{n,k,i} - |M| q_{c,M}^n,$$

where $F_{c,M,\sigma}^{n,k,i}$ is a linearized component flux

Linearization and algebraic resolution III

Corollary (Time-localized a posteriori error estimate)

For a given time step n, Newton iteration k, and linear iteration i we have

$$\mathcal{N}_c^n \leq \left\{ \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{R},M,c}^{n,k,i} + \eta_{\mathrm{F},M,c}^{n,k,i}(t) + \eta_{\mathrm{NA},M,c}^{n,k,i} \right)^2 \mathrm{d}t \right\}^{1/2} \quad \forall c \in \mathcal{C},$$

$$\mathcal{N}_p^n \leq \left\{ \sum_{c \in \mathcal{C}_p} \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta_{\mathrm{NC},M,p,c}^{n,k,i}(t) \right)^2 \mathrm{d}t \right\}^{1/2} \quad \forall p \in \mathcal{P},$$

where $\eta_{\mathrm{NA},M,c}^{n,k,i}$ is related to the nonlinear accumulation term.

Distinguishing the error components I

- We decompose the component flux reconstruction $\mathbf{\Theta}_{c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ as

$$\boxed{\mathbf{\Theta}_{c,h}^{n,k,i} := \mathbf{\Theta}_{\mathrm{disc},c,h}^{n,k,i} + \mathbf{\Theta}_{\mathrm{lin},c,h}^{n,k,i} + \mathbf{\Theta}_{\mathrm{alg},c,h}^{n,k,i}}$$

- The discretization flux reconstruction $\mathbf{\Theta}_{\mathrm{disc},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ is s.t.

$$(\mathbf{\Theta}_{\mathrm{disc},c,h}^{n,k,i} \cdot \boldsymbol{n}_M, 1)_\sigma := F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i})$$

- The linearization error flux reconstruction $\mathbf{\Theta}_{\mathrm{lin},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ is s.t.

$$(\mathbf{\Theta}_{\mathrm{lin},c,h}^{n,k,i} \cdot \boldsymbol{n}_M, 1)_\sigma = F_{c,M,\sigma}^{n,k,i} - F_{c,M,\sigma}(\mathcal{X}_{\mathcal{M}}^{n,k,i})$$

- The algebraic error flux reconstruction $\mathbf{\Theta}_{\mathrm{alg},c,h}^{n,k,i} \in \mathbf{RTN}(\mathcal{M}^n)$ is s.t.

$$(\mathbf{\Theta}_{\mathrm{alg},c,h}^{n,k,i} \cdot \boldsymbol{n}_M, 1)_{\partial M} := -R_{c,M}^{n,k,i}$$

Distinguishing the error components II

- Space error estimator

$$\eta_{\mathrm{sp},M,c}^{n,k,i}(t) := \eta_{\mathrm{R},M,c}^{n,k,i} + \|\boldsymbol{\Theta}_{\mathrm{disc},c,h}^{n,k,i} - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t^n)\|_M + \left\{ \sum_{p\in\mathcal{P}_c} \left(\eta_{\mathrm{NC},M,p,c}^{n,k,i}(t)\right)^2 \right\}^{1/2}$$

- Time error estimator

$$\eta_{\mathrm{tm},M,c}^{n,k,i}(t) := \|\boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t^n) - \boldsymbol{\Phi}_{c,h\tau}^{n,k,i}(t)\|_M$$

- Linearization error estimator

$$\eta_{\mathrm{lin},M,c}^{n,k,i} := \|\boldsymbol{\Theta}_{\mathrm{lin},c,h}^{n,k,i}{}_M\| + \eta_{\mathrm{NA},M,c}^{n,k,i}$$

- Algebraic error estimator

$$\eta_{\mathrm{alg},M,c}^{n,k,i} := \|\boldsymbol{\Theta}_{\mathrm{alg},c,h}^{n,k,i}\|_M$$

Distinguishing the error components III

Corollary (Distinguishing the different error components)

The following estimate holds:

$$\mathcal{N}^n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta^{n,k,i}_{\mathrm{sp},c} + \eta^{n,k,i}_{\mathrm{tm},c} + \eta^{n,k,i}_{\mathrm{lin},c} + \eta^{n,k,i}_{\mathrm{alg},c} \right)^2 \right\}^{1/2},$$

with estimators given by

$$\eta^{n,k,i}_{\mathrm{sp},c} := \left\{ 4 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta^{n,k,i}_{\mathrm{sp},M,c}(t) \right)^2 \mathrm{d}t \right\}^{1/2},$$

$$\eta^{n,k,i}_{\mathrm{tm},c} := \left\{ 2 \int_{I_n} \sum_{M \in \mathcal{M}^n} \left(\eta^{n,k,i}_{\mathrm{tm},M,c}(t) \right)^2 \mathrm{d}t \right\}^{1/2},$$

$$\eta^{n,k,i}_{\mathrm{lin},c} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta^{n,k,i}_{\mathrm{lin},M,c} \right)^2 \right\}^{1/2},$$

$$\eta^{n,k,i}_{\mathrm{alg},c} := \left\{ 2\tau^n \sum_{M \in \mathcal{M}^n} \left(\eta^{n,k,i}_{\mathrm{alg},M,c} \right)^2 \right\}^{1/2}.$$

A fully adaptive algorithm

Fix $\mathcal{M}^0$ and τ_0. Set $t^0 \leftarrow 0$, $n \leftarrow 0$ and set the initial solution $\mathcal{X}_{h\tau}^0$.
while $t^n \leq t^F$ **do**
Set $n \leftarrow n+1$, $\mathcal{M}^n \leftarrow \mathcal{M}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$.
repeat { Equilibration of spatial and temporal errors }
Set $k \leftarrow 0$ and $\mathcal{X}_{h\tau}^{n,0} \leftarrow \mathcal{X}_{h\tau}^{n-1}$.
repeat { Newton iterations }
$k \leftarrow k+1$ and $i \leftarrow 0$. Set $\mathcal{X}_{h\tau}^{n,k,0} := \mathcal{X}_{h\tau}^{n,k-1}$.
Set up the linear system
repeat { Algebraic iterations }
Set $i = i+1$ and perform one iteration of the algebraic solver
Compute $\eta_{\mathrm{sp}}^{n,k,i}$, $\eta_{\mathrm{tm}}^{n,k,i}$, $\eta_{\mathrm{lin}}^{n,k,i}$, $\eta_{\mathrm{alg}}^{n,k,i}$

until

until

Adapt the time step τ^n

until

Set $\mathcal{X}_{h\tau}^n \leftarrow \mathcal{X}_{h\tau}^{n,k,i}$, and $t^n \leftarrow t^{n-1} + \tau^n$.
end while

A fully adaptive algorithm

Fix $\mathcal{M}^0$ and τ_0. Set $t^0 \leftarrow 0$, $n \leftarrow 0$ and set the initial solution $\mathcal{X}_{h\tau}^0$.
while $t^n \leq t^F$ **do**
  Set $n \leftarrow n+1$, $\mathcal{M}^n \leftarrow \mathcal{M}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$.
  repeat { Equilibration of spatial and temporal errors }
    Set $k \leftarrow 0$ and $\mathcal{X}_{h\tau}^{n,0} \leftarrow \mathcal{X}_{h\tau}^{n-1}$.
    repeat { Newton iterations }
      $k \leftarrow k+1$ and $i \leftarrow 0$. Set $\mathcal{X}_{h\tau}^{n,k,0} := \mathcal{X}_{h\tau}^{n,k-1}$.
      Set up the linear system
      repeat { Algebraic iterations }
        Set $i = i+1$ and perform one iteration of the algebraic solver
        Compute $\eta_{\mathrm{sp}}^{n,k,i}$, $\eta_{\mathrm{tm}}^{n,k,i}$, $\eta_{\mathrm{lin}}^{n,k,i}$, $\eta_{\mathrm{alg}}^{n,k,i}$
      until $\eta_{\mathrm{alg},c}^{n,k,i} \leq \gamma_{\mathrm{alg}}(\eta_{\mathrm{sp},c}^{n,k,i} + \eta_{\mathrm{tm},c}^{n,k,i} + \eta_{\mathrm{lin},c}^{n,k,i}) \quad \forall c \in \mathcal{C}$
    until
    Adapt the time step τ^n
  until
  Set $\mathcal{X}_{h\tau}^n \leftarrow \mathcal{X}_{h\tau}^{n,k,i}$, and $t^n \leftarrow t^{n-1} + \tau^n$.
end while

A fully adaptive algorithm

Fix $\mathcal{M}^0$ and τ_0. Set $t^0 \leftarrow 0$, $n \leftarrow 0$ and set the initial solution $\mathcal{X}_{h\tau}^0$.
while $t^n \leq t^F$ **do**
  Set $n \leftarrow n+1$, $\mathcal{M}^n \leftarrow \mathcal{M}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$.
  repeat { Equilibration of spatial and temporal errors }
    Set $k \leftarrow 0$ and $\mathcal{X}_{h\tau}^{n,0} \leftarrow \mathcal{X}_{h\tau}^{n-1}$.
    repeat { Newton iterations }
      $k \leftarrow k+1$ and $i \leftarrow 0$. Set $\mathcal{X}_{h\tau}^{n,k,0} := \mathcal{X}_{h\tau}^{n,k-1}$.
      Set up the linear system
      repeat { Algebraic iterations }
        Set $i = i+1$ and perform one iteration of the algebraic solver
        Compute $\eta_{\rm sp}^{n,k,i}$, $\eta_{\rm tm}^{n,k,i}$, $\eta_{\rm lin}^{n,k,i}$, $\eta_{\rm alg}^{n,k,i}$
      until $\eta_{{\rm alg},c}^{n,k,i} \leq \gamma_{\rm alg}(\eta_{{\rm sp},c}^{n,k,i} + \eta_{{\rm tm},c}^{n,k,i} + \eta_{{\rm lin},c}^{n,k,i}) \quad \forall c \in \mathcal{C}$
    until $\eta_{{\rm lin},c}^{n,k,i} \leq \gamma_{\rm lin}(\eta_{{\rm sp},c}^{n,k,i} + \eta_{{\rm tm},c}^{n,k,i}) \quad \forall c \in \mathcal{C}$
    Adapt the time step τ^n
  until
  Set $\mathcal{X}_{h\tau}^n \leftarrow \mathcal{X}_{h\tau}^{n,k,i}$, and $t^n \leftarrow t^{n-1} + \tau^n$.
end while

A fully adaptive algorithm

Fix $\mathcal{M}^0$ and τ_0. Set $t^0 \leftarrow 0$, $n \leftarrow 0$ and set the initial solution $\mathcal{X}^0_{h\tau}$.
while $t^n \leq t^F$ **do**
  Set $n \leftarrow n+1$, $\mathcal{M}^n \leftarrow \mathcal{M}^{n-1}$, $\tau^n \leftarrow \tau^{n-1}$.
  repeat { Equilibration of spatial and temporal errors }
    Set $k \leftarrow 0$ and $\mathcal{X}^{n,0}_{h\tau} \leftarrow \mathcal{X}^{n-1}_{h\tau}$.
    repeat { Newton iterations }
      $k \leftarrow k+1$ and $i \leftarrow 0$. Set $\mathcal{X}^{n,k,0}_{h\tau} := \mathcal{X}^{n,k-1}_{h\tau}$.
      Set up the linear system
      repeat { Algebraic iterations }
        Set $i = i+1$ and perform one iteration of the algebraic solver
        Compute $\eta^{n,k,i}_{\mathrm{sp}}$, $\eta^{n,k,i}_{\mathrm{tm}}$, $\eta^{n,k,i}_{\mathrm{lin}}$, $\eta^{n,k,i}_{\mathrm{alg}}$
      until $\eta^{n,k,i}_{\mathrm{alg},c} \leq \gamma_{\mathrm{alg}}(\eta^{n,k,i}_{\mathrm{sp},c} + \eta^{n,k,i}_{\mathrm{tm},c} + \eta^{n,k,i}_{\mathrm{lin},c}) \quad \forall c \in \mathcal{C}$
    until $\eta^{n,k,i}_{\mathrm{lin},c} \leq \gamma_{\mathrm{lin}}(\eta^{n,k,i}_{\mathrm{sp},c} + \eta^{n,k,i}_{\mathrm{tm},c}) \quad \forall c \in \mathcal{C}$
    Adapt the time step τ^n
  until $\gamma_{\mathrm{tm}}\eta^{n,k,i}_{\mathrm{sp},c} \leq \eta^{n,k,i}_{\mathrm{tm},c} \leq \Gamma_{\mathrm{tm}}\eta^{n,k,i}_{\mathrm{sp},c} \quad \forall c \in \mathcal{C}$
  Set $\mathcal{X}^n_{h\tau} \leftarrow \mathcal{X}^{n,k,i}_{h\tau}$, and $t^n \leftarrow t^{n-1} + \tau^n$.
end while

Adaptive stopping criteria

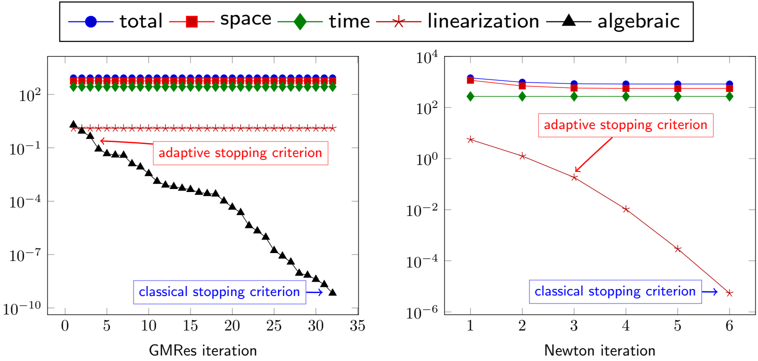

Figure: Evolution of the error component estimators for a fixed mesh as a function of GMRes (left) and Newton iterations (right)

Outline

A numerical example

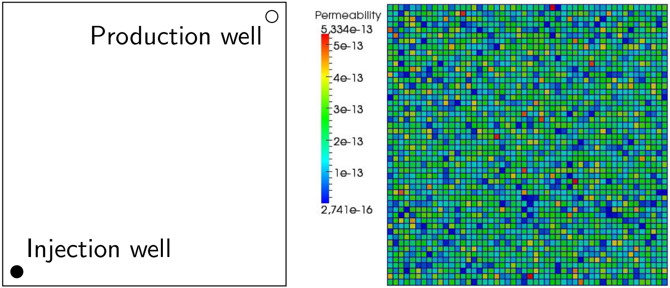

Figure: Numerical example: injection of a mixture of CO_2 and N_2 into a reservoir initially saturated with C_7H_{16}

Homogeneous medium I

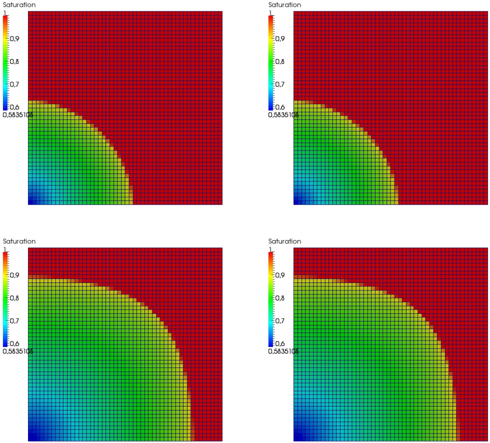

Figure: Liquid saturation, classical (left) vs. adaptive (right) resolution at times 7.8×10^7 s and 2.1×10^8 s

Homogeneous medium II

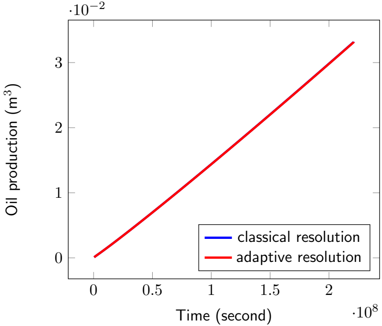

Figure: Cumulated oil production, classical vs. adaptive resolution

Homogeneous medium III

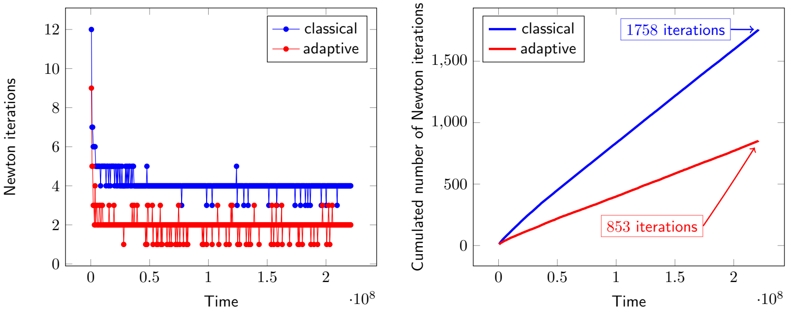

Figure: Newton iterations at each time step (left) and cumulated number of Newton iterations as a function of time (right).

Homogeneous medium IV

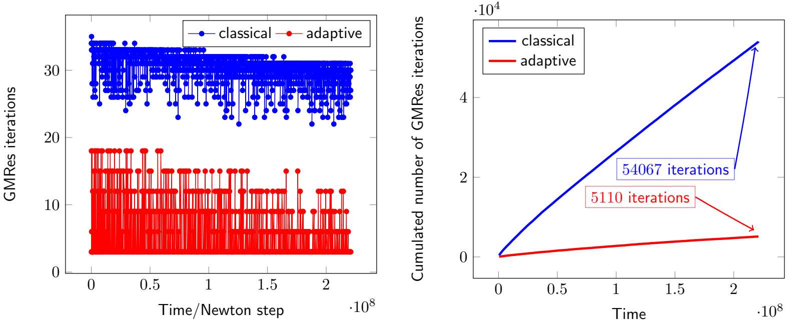

Figure: GMRes iterations for each Newton iteration (left) and cumulated as a function of time (right)

Heterogeneous medium I

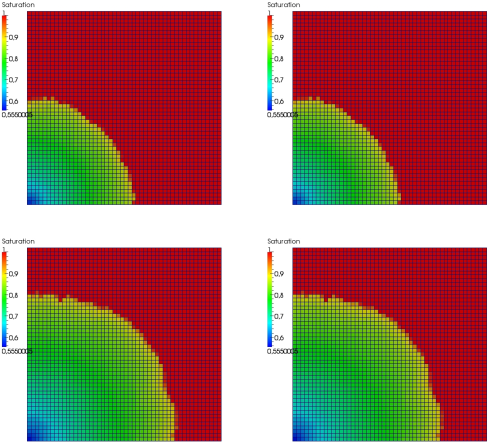

Figure: Liquid saturation, classical (left) and adaptive (right) resolutions at times 5.2×10^7 s, 1.04×10^8 s, and 1.6×10^8 s (heterogeneous medium)

Heterogeneous medium II

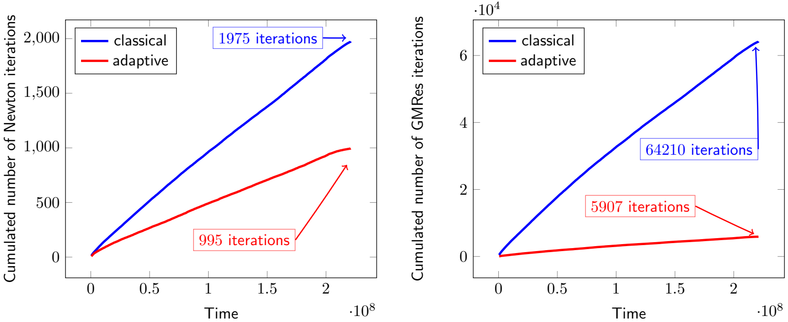

Figure: Cumulated Newton (left) and GMRes (right) iterations as a function of time (right) (heterogeneous medium)

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