Adaptive inexact Newton methods and their application to multi-phase flows

Martin Vohralík

INRIA Paris-Rocquencourt

in collaboration with Clément Cancès, Daniele A. Di Pietro, Alexandre Ern, Eric Flauraud, I. Sorin Pop, Mary F. Wheeler, and Soleiman Yousef

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Outline

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2. Adaptive inexact Newton method
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3. Application to two-phase flow in porous media
   - A guaranteed a posteriori error estimate
   - Application and numerical results
4. Application to multi-phase flow in porous media
   - A guaranteed a posteriori error estimate
   - Application and numerical results
5. Conclusions and future directions

Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator $\mathcal{A}:\mathbb{R}^N \to \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

$$\mathcal{A}(U) = F$$

Algorithm (Inexact iterative linearization)

1. *Choose initial vector* U^0. *Set* $k := 1$.
2. $U^{k-1} \Rightarrow$ *matrix* $\mathbb{A}^{k-1}$ *and vector* F^{k-1}: *find* U^k *s.t.*
$$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$
3.
   1. *Set* $U^{k,0} := U^{k-1}$ *and* $i := 1$.
   2. *Do* 1 *algebraic solver step* $\Rightarrow U^{k,i}$ *s.t.* ($R^{k,i}$ *algebraic res.*)
   $$\mathbb{A}^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.$$
   3. *Convergence? OK* $\Rightarrow U^k := U^{k,i}$. *KO* $\Rightarrow i := i + 1$, *back to 3.2.*
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Context and questions

Approximate solution

- approximate solution $U^{k,i}$ does not solve $\mathcal{A}(U^{k,i}) = F$

Numerical method

- underlying numerical method: the vector $U^{k,i}$ is associated with a (piecewise polynomial) approximation $u_h^{k,i}$

Partial differential equation

- underlying PDE, u its weak solution: $A(u) = f$

Question (Stopping criteria)

- *What is a good stopping criterion for the linear solver?*
- *What is a good stopping criterion for the nonlinear solver?*

Question (Error)

- *How big is the error $\|u - u_h^{k,i}\|$ on Newton step k and algebraic solver step i, how is it distributed?*

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Inexact Newton method

- Eisenstat and Walker (1990's) (conception, convergence, a priori error estimates)
- Moret (1989) (discrete a posteriori error estimates)

Adaptive inexact Newton method

- Bank and Rose (1982), combination with multigrid
- Hackbusch and Reusken (1989), damping and multigrid
- Deuflhard (1990's, 2004 book), adaptivity

Stopping criteria for algebraic solvers

- engineering literature, since 1950's
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A posteriori error estimates for numerical discretizations of nonlinear problems

- Ladevèze (since 1990's), guaranteed upper bound
- Han (1994), general framework
- Verfürth (1994), residual estimates
- Carstensen and Klose (2003), guaranteed estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors
- Kim (2007), guaranteed estimates, locally conservative methods

Outline

Quasi-linear elliptic problem

Quasi-linear elliptic problem

$$-\nabla\cdot\sigma(u,\nabla u) = f \qquad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega$$

- quasi-linear diffusion problem

$$\sigma(v,\xi) = \underline{\mathbf{A}}(v)\xi \qquad \forall (v,\xi) \in \mathbb{R}\times\mathbb{R}^d$$

- Leray–Lions problem

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- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$

Example

p-Laplacian: Leray–Lions setting with $\underline{\mathbf{A}}(\xi) = |\xi|^{p-2}\underline{\mathbf{I}}$

Nonlinear operator $A : V := W_0^{1,p}(\Omega) \to V'$

$$\langle A(u), v\rangle_{V',V} := (\sigma(u,\nabla u), \nabla v)$$

Weak formulation

Find $u \in V$ such that

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- $u_h^{k,i} \in V(\mathcal{T}_h) \not\subset V$, $u_h^{k,i}$ not necessarily in V
- $V(\mathcal{T}_h) := \{v \in L^p(\Omega),\ v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\}$

Error measure

$$\mathcal{J}_u(u_h^{k,i}) := \sup_{\varphi \in V;\, \|\nabla\varphi\|_p = 1} (\sigma(u,\nabla u) - \sigma(u_h^{k,i}, \nabla u_h^{k,i}), \nabla\varphi) + \mathcal{J}_{u,\mathrm{NC}}(u_h^{k,i})$$

$$\mathcal{J}_{u,\mathrm{NC}}(u_h^{k,i}) := \left\{ \sum_{K \in \mathcal{T}_h} \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u - u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}}$$

- dual norm of the residual + nonconformity
- there holds $\mathcal{J}_u(u_h^{k,i}) = 0$ if and only if $u = u_h^{k,i}$
- link: **strong** difference of the **fluxes** + **nonconformity**

$$\mathcal{J}_u(u_h^{k,i}) \le \mathcal{J}_u^{\mathrm{up}}(u_h^{k,i}) := \|\sigma(u, \nabla u) - \sigma(u_h^{k,i}, \nabla u_h^{k,i})\|_q + \mathcal{J}_{u,\mathrm{NC}}(u_h^{k,i})$$

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$$\mathcal{J}_{u,\mathrm{NC}}(u_h^{k,i}) := \left\{ \sum_{K \in \mathcal{T}_h} \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u - u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}}$$

- dual norm of the residual + nonconformity
- there holds $\mathcal{J}_u(u_h^{k,i}) = 0$ if and only if $u = u_h^{k,i}$
- link: **strong** difference of the **fluxes** + **nonconformity**

$$\mathcal{J}_u(u_h^{k,i}) \le \mathcal{J}_u^{\mathrm{up}}(u_h^{k,i}) := \|\boldsymbol{\sigma}(u,\nabla u) - \boldsymbol{\sigma}(u_h^{k,i},\nabla u_h^{k,i})\|_q + \mathcal{J}_{u,\mathrm{NC}}(u_h^{k,i})$$

Approximate solution and error measure

Approximate solution

- $u_h^{k,i} \in V(\mathcal{T}_h) \not\subset V$, $u_h^{k,i}$ not necessarily in V
- $V(\mathcal{T}_h) := \{v \in L^p(\Omega),\ v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\}$

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Outline

A posteriori error estimate

Assumption A (Total quasi-equilibrated flux reconstruction)

There exists a flux reconstruction $\mathbf{t}_h^{k,i} \in \mathbf{H}^q(\mathrm{div}, \Omega)$ *and an algebraic remainder* $\rho_h^{k,i} \in L^q(\Omega)$ *such that*

$$\nabla\cdot\mathbf{t}_h^{k,i} = f_h - \rho_h^{k,i},$$

with the data approximation f_h *s.t.* $(f_h, 1)_K = (f, 1)_K \;\; \forall K \in \mathcal{T}_h$.

Theorem (A guaranteed a posteriori error estimate)

Let

- $u \in V$ *be the weak solution,*
- $u_h^{k,i} \in V(\mathcal{T}_h)$ *be arbitrary,*
- *Assumption A hold.*

Then there holds

$$\mathcal{J}_u(u_h^{k,i}) \leq \overline{\eta}^{k,i},$$

where $\overline{\eta}^{k,i}$ *is fully computable from* $u_h^{k,i}$, $\mathbf{t}_h^{k,i}$, *and* $\rho_h^{k,i}$.

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Distinguishing error components

Assumption B (Discretization, linearization, and algebraic errors)

There exist fluxes $\mathbf{d}_h^{k,i}, \mathbf{l}_h^{k,i}, \mathbf{a}_h^{k,i} \in [L^q(\Omega)]^d$ *such that*

(i) $\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i} + \mathbf{a}_h^{k,i} = \mathbf{t}_h^{k,i}$;

(ii) *as the linear solver converges,* $\|\mathbf{a}_h^{k,i}\|_q \to 0$;

(iii) *as the nonlinear solver converges,* $\|\mathbf{l}_h^{k,i}\|_q \to 0$.

Comments

- $\mathbf{d}_h^{k,i}$: *discretization flux reconstruction*
- $\mathbf{l}_h^{k,i}$: *linearization* ***error*** *flux reconstruction*
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Estimate distinguishing error components

Theorem (Estimate distinguishing different error components)

Let

- $u \in V$ *be the weak solution,*
- $u_h^{k,i} \in V(\mathcal{T}_h)$ *be arbitrary,*
- *Assumptions A and B hold.*

Then there holds

$$\mathcal{J}_u(u_h^{k,i}) \leq \eta^{k,i} := \eta_{\rm disc}^{k,i} + \eta_{\rm lin}^{k,i} + \eta_{\rm alg}^{k,i} + \eta_{\rm rem}^{k,i} + \eta_{\rm quad}^{k,i} + \eta_{\rm osc}^{k,i}.$$

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Estimators

- *discretization* estimator

$$\eta_{\mathrm{disc},K}^{k,i} := 2^{\frac{1}{p}} \left(\|\overline{\boldsymbol{\sigma}}_h^{k,i} + \mathbf{d}_h^{k,i}\|_{q,K} + \left\{ \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}} \right)$$

- *linearization* estimator

$$\eta_{\mathrm{lin},K}^{k,i} := \|\mathbf{l}_h^{k,i}\|_{q,K}$$

- *algebraic* estimator

$$\eta_{\mathrm{alg},K}^{k,i} := \|\mathbf{a}_h^{k,i}\|_{q,K}$$

- *algebraic remainder estimator*

$$\eta_{\mathrm{rem},K}^{k,i} := h_\Omega \|\rho_h^{k,i}\|_{q,K}$$

- *quadrature estimator*

$$\eta_{\mathrm{quad},K}^{k,i} := \|\boldsymbol{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}) - \overline{\boldsymbol{\sigma}}_h^{k,i}\|_{q,K}$$

- *data oscillation estimator*

$$\eta_{\mathrm{osc},K}^{k,i} := C_{\mathrm{P},p} h_K \|f - f_h\|_{q,K}$$

- $\eta_{\cdot}^{k,i} := \left\{ \sum_{K \in \mathcal{T}_h} (\eta_{\cdot,K}^{k,i})^q \right\}^{1/q}$

Outline

Stopping criteria

Global stopping criteria

- stop whenever:

$$\eta_{\mathrm{rem}}^{k,i} \leq \gamma_{\mathrm{rem}} \max\{\eta_{\mathrm{disc}}^{k,i}, \eta_{\mathrm{lin}}^{k,i}, \eta_{\mathrm{alg}}^{k,i}\},$$
$$\eta_{\mathrm{alg}}^{k,i} \leq \gamma_{\mathrm{alg}} \max\{\eta_{\mathrm{disc}}^{k,i}, \eta_{\mathrm{lin}}^{k,i}\},$$
$$\eta_{\mathrm{lin}}^{k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i}$$

- $\gamma_{\mathrm{rem}}, \gamma_{\mathrm{alg}}, \gamma_{\mathrm{lin}} \approx 0.1$

Local stopping criteria

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$$\eta_{\mathrm{alg},K}^{k,i} \leq \gamma_{\mathrm{alg},K} \max\{\eta_{\mathrm{disc},K}^{k,i}, \eta_{\mathrm{lin},K}^{k,i}\} \qquad \forall K \in \mathcal{T}_h,$$
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Assumption for efficiency

Assumption C (Approximation property)

For all $K \in \mathcal{T}_h$, there holds

$$\|\overline{\boldsymbol{\sigma}}_h^{k,i} + \mathbf{d}_h^{k,i}\|_{q,K} \lesssim \eta_{\sharp,\mathfrak{T}_K}^{k,i} + \eta_{\mathrm{osc},\mathfrak{T}_K}^{k,i},$$

where

$$\eta_{\sharp,\mathfrak{T}_K}^{k,i} := \left\{ \sum_{K' \in \mathfrak{T}_K} h_{K'}^q \|f_h + \nabla\cdot\overline{\boldsymbol{\sigma}}_h^{k,i}\|_{q,K'}^q + \sum_{e \in \mathfrak{E}_K^{\mathrm{int}}} h_e \|[\![\overline{\boldsymbol{\sigma}}_h^{k,i}\cdot\mathbf{n}_e]\!]\|_{q,e}^q + \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}}.$$

Global efficiency

Theorem (Global efficiency)

Let the mesh $\mathcal{T}_h$ be shape-regular and let the global stopping criteria hold. Recall that $\mathcal{J}_u(u_h^{k,i}) \leq \eta^{k,i}$. Then, under Assumption C,

$$\eta^{k,i} \lesssim \mathcal{J}_u(u_h^{k,i}) + \eta_{\mathrm{quad}}^{k,i} + \eta_{\mathrm{osc}}^{k,i},$$

where $\lesssim$ means up to a constant independent of σ and q.

- **robustness** with respect to the **nonlinearity** thanks to the choice of the dual norm as error measure

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Outline

Algebraic error flux reconstruction and remainder

Construction of $\mathbf{a}_h^{k,i}$ and $\rho_h^{k,i}$

- On linearization step k and algebraic step i, we have

$$\mathbb{A}^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.$$

- Do ν additional steps of the algebraic solver, yielding

$$\mathbb{A}^{k-1} U^{k,i+\nu} = F^{k-1} - R^{k,i+\nu}.$$

- Construct the function $\rho_h^{k,i}$ from the algebraic residual vector $R^{k,i+\nu}$ (lifting into appropriate discrete space).
- Suppose we can obtain discretization and linearization flux reconstructions $\mathbf{d}_h^{k,i}, \mathbf{l}_h^{k,i}$ on each algebraic step. Then set

$$\mathbf{a}_h^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}).$$

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Nonconforming finite elements for the p-Laplacian

Discretization

Find $u_h \in V_h$ such that

$$(\boldsymbol{\sigma}(\nabla u_h), \nabla v_h) = (f_h, v_h) \qquad \forall v_h \in V_h.$$

- $\boldsymbol{\sigma}(\nabla u_h) = |\nabla u_h|^{p-2} \nabla u_h$
- V_h the Crouzeix–Raviart space
- $f_h := \Pi_0 f$
- leads to the system of nonlinear algebraic equations

$$\mathcal{A}(U) = F$$

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Linearization

Linearization

Find $u_h^k \in V_h$ such that

$$(\boldsymbol{\sigma}^{k-1}(\nabla u_h^k), \nabla \psi_e) = (f_h, \psi_e) \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}.$$

- $u_h^0 \in V_h$ yields the initial vector U^0
- fixed-point linearization

$$\boldsymbol{\sigma}^{k-1}(\boldsymbol{\xi}) := |\nabla u_h^{k-1}|^{p-2} \boldsymbol{\xi}$$

- Newton linearization

$$\boldsymbol{\sigma}^{k-1}(\boldsymbol{\xi}) := |\nabla u_h^{k-1}|^{p-2} \boldsymbol{\xi} + (p-2) |\nabla u_h^{k-1}|^{p-4} (\nabla u_h^{k-1} \otimes \nabla u_h^{k-1})(\boldsymbol{\xi} - \nabla u_h^{k-1})$$

- leads to the system of linear algebraic equations

$$\mathbb{A}^{k-1} U^k = F^{k-1}$$

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Linearization

Find $u_h^k \in V_h$ such that

$$(\boldsymbol{\sigma}^{k-1}(\nabla u_h^k), \nabla \psi_e) = (f_h, \psi_e) \qquad \forall e \in \mathcal{E}_h^{\text{int}}.$$

- $u_h^0 \in V_h$ yields the initial vector U^0
- fixed-point linearization

$$\boldsymbol{\sigma}^{k-1}(\boldsymbol{\xi}) := |\nabla u_h^{k-1}|^{p-2}\boldsymbol{\xi}$$

- Newton linearization

$$\boldsymbol{\sigma}^{k-1}(\boldsymbol{\xi}) := |\nabla u_h^{k-1}|^{p-2}\boldsymbol{\xi} + (p-2)|\nabla u_h^{k-1}|^{p-4} (\nabla u_h^{k-1} \otimes \nabla u_h^{k-1})(\boldsymbol{\xi} - \nabla u_h^{k-1})$$

- leads to the system of linear algebraic equations

$$\mathbb{A}^{k-1} U^k = F^{k-1}$$

Algebraic solution

Algebraic solution

Find $u_h^{k,i} \in V_h$ such that

$$(\boldsymbol{\sigma}^{k-1}(\nabla u_h^{k,i}), \nabla \psi_e) = (f_h, \psi_e) - R_e^{k,i} \qquad \forall e \in \mathcal{E}_h^{\mathrm{int}}.$$

- algebraic residual vector $R^{k,i} = \{R_e^{k,i}\}_{e \in \mathcal{E}_h^{\mathrm{int}}}$
- discrete system

$$\mathbb{A}^{k-1} U^k = F^{k-1} - R^{k,i}$$

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Flux reconstructions

Definition (Construction of $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i})$)

For all $K \in \mathcal{T}_h$,

$$(\mathbf{d}_h^{k,i}+\mathbf{l}_h^{k,i})|_K := -\boldsymbol{\sigma}^{k-1}(\nabla u_h^{k,i})|_K + \frac{f_h|_K}{d}(\mathbf{x}-\mathbf{x}_K) - \sum_{e\in\mathcal{E}_K} \frac{R_e^{k,i}}{d|D_e|}(\mathbf{x}-\mathbf{x}_K)|_{K_e},$$

where, $R_e^{k,i} = (f_h, \psi_e) - (\boldsymbol{\sigma}^{k-1}(\nabla u_h^{k,i}), \nabla\psi_e) \qquad \forall e \in \mathcal{E}_h^{\text{int}}$.

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Set $\overline{\boldsymbol{\sigma}}_h^{k,i} := \boldsymbol{\sigma}(\nabla u_h^{k,i})$. Consequently, $\eta_{\text{quad},K}^{k,i} = 0$ for all $K \in \mathcal{T}_h$.

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Verification of the assumptions – upper bound

Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

- $\|\mathbf{a}_h^{k,i}\|_{q,K} \to 0$ as the linear solver converges by definition.
- $\|\mathbf{l}_h^{k,i}\|_{q,K} \to 0$ as the nonlinear solver converges by the construction of $\mathbf{l}_h^{k,i}$.
- Both $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i})$ and $\mathbf{d}_h^{k,i}$ belong to $\mathbf{RTN}_0(\mathcal{S}_h) \Rightarrow$ $\mathbf{a}_h^{k,i} \in \mathbf{RTN}_0(\mathcal{S}_h)$ and $\mathbf{t}_h^{k,i} \in \mathbf{RTN}_0(\mathcal{S}_h)$.

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Verification of the assumptions – efficiency

Lemma (Assumption C)

Assumption C holds.

Comments

- $\mathbf{d}_h^{k,i}$ close to $\sigma(\nabla u_h^{k,i})$
- approximation properties of Raviart–Thomas–Nédélec spaces

Verification of the assumptions – efficiency

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Assumption C holds.

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- approximation properties of Raviart–Thomas–Nédélec spaces

Summary

Discretization methods

- conforming finite elements
- nonconforming finite elements
- discontinuous Galerkin
- various finite volumes
- mixed finite elements

Linearizations

- fixed point
- Newton

Linear solvers

- independent of the linear solver

. . . all Assumptions A to C verified

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Numerical experiment I

Model problem

- p-Laplacian

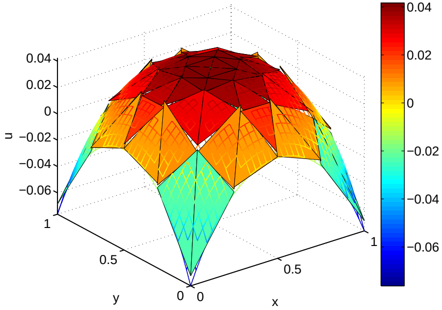
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f \quad \text{in } \Omega, \\ u &= u_{\mathrm{D}} \quad \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

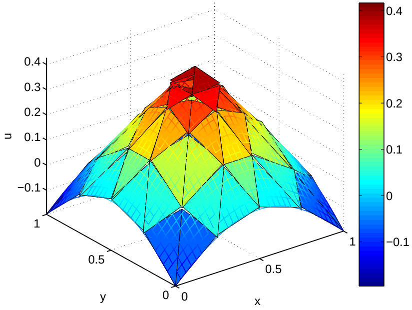
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

- tested values $p = 1.5$ and 10
- nonconforming finite elements

Analytical and approximate solutions

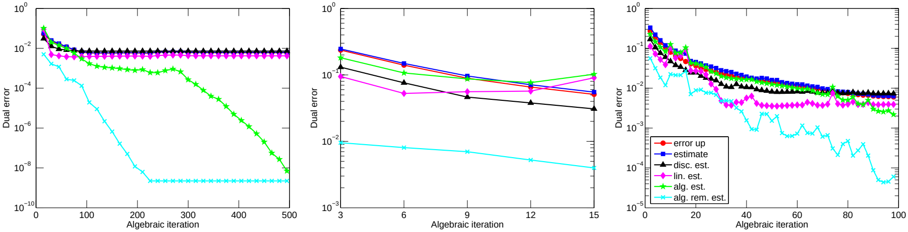


Case $p = 1.5$



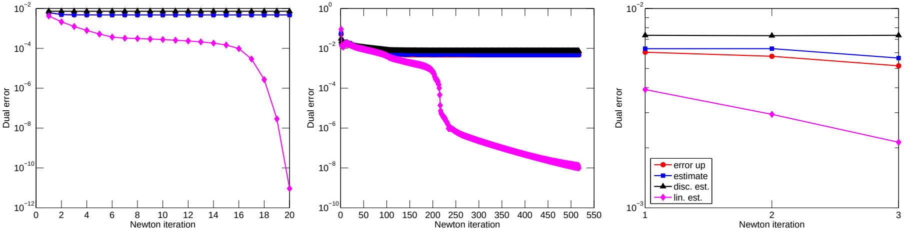
Case $p = 10$

Error and estimators as a function of CG iterations, $p = 1.5$, 6th level mesh, 1st Newton step.



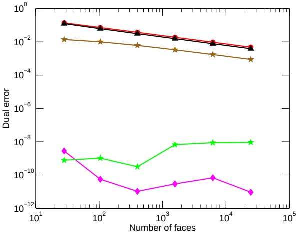
Newton inexact Newton ad. inexact Newton

Error and estimators as a function of Newton iterations, $p = 1.5$, 6th level mesh

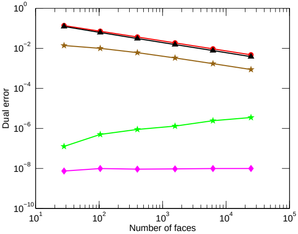


Newton | inexact Newton | ad. inexact Newton

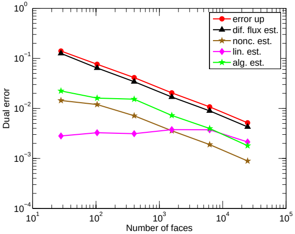
Error and estimators, $p = 1.5$



Newton

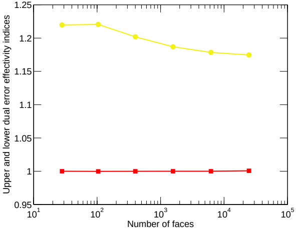


inexact Newton

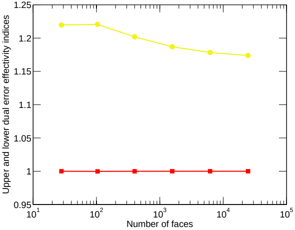


ad. inexact Newton

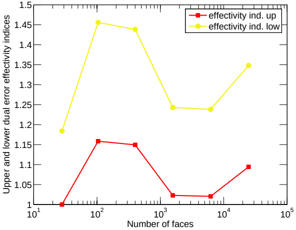
Effectivity indices, $p = 1.5$



Newton

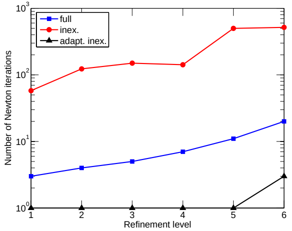


inexact Newton

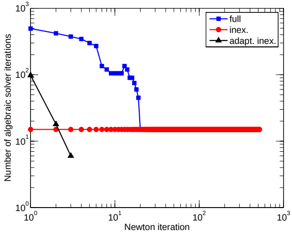


ad. inexact Newton

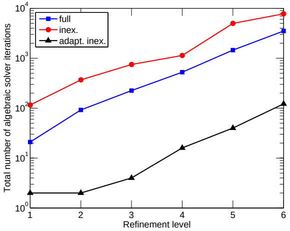
Newton and algebraic iterations, $p = 1.5$



Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p-Laplacian

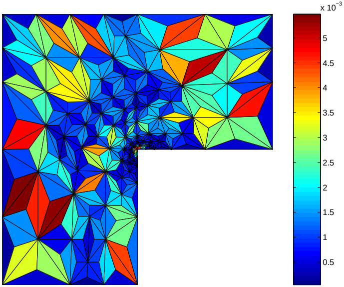
$$\nabla\cdot(|\nabla u|^{p-2}\nabla u) = f \quad \text{in } \Omega,$$
$$u = u_{\mathrm{D}} \quad \text{on } \partial\Omega$$

- weak solution (used to impose the Dirichlet BC)

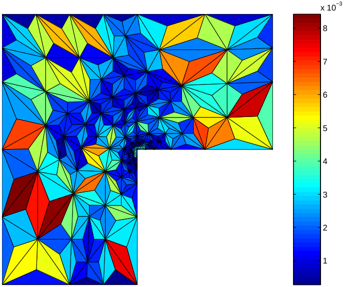
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

- $p = 4$, L-shape domain, singularity in the origin (Carstensen and Klose (2003))
- nonconforming finite elements

Error distribution on an adaptively refined mesh

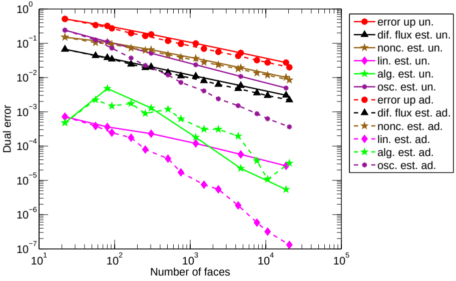


Estimated error distribution

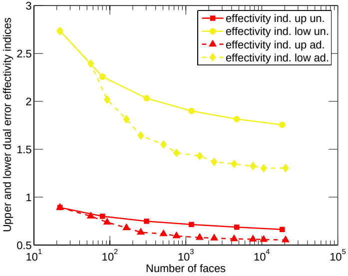


Exact error distribution

Estimated and actual errors and the effectivity index

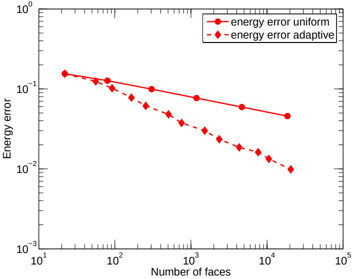


Estimated and actual errors

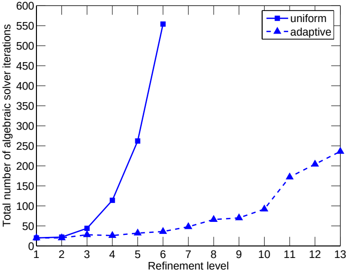


Effectivity index

Energy error and overall performance



Energy error



Overall performance

Outline

Two-phase flow in porous media

Two-phase flow in porous media

$$
\begin{aligned}
\partial_t(\phi s_\alpha) + \nabla\cdot\mathbf{u}_\alpha &= q_\alpha, & \alpha &\in \{\mathrm{n}, \mathrm{w}\},\\
-\lambda_\alpha(s_\mathrm{w})\underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha g \nabla z) &= \mathbf{u}_\alpha, & \alpha &\in \{\mathrm{n}, \mathrm{w}\},\\
s_\mathrm{n} + s_\mathrm{w} &= 1,\\
p_\mathrm{n} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w})
\end{aligned}
$$

+ boundary & initial conditions

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–degenerate parabolic type
- dominant advection

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Global and complementary pressures

Global pressure

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

Complementary pressure

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

Comments

- necessary for the correct definition of the weak solution
- equivalent Darcy velocities expressions

$$\mathbf{u}_{\rm w}(s_{\rm w}, p_{\rm w}) := -\underline{\mathbf{K}}\big(\lambda_{\rm w}(s_{\rm w})\nabla\mathfrak{p}(s_{\rm w}, p_{\rm w}) + \nabla\mathfrak{q}(s_{\rm w}) + \lambda_{\rm w}(s_{\rm w})\rho_{\rm w} g\nabla z\big),$$
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Weak formulation

Energy space

$$X := L^2((0,T); H^1_{\mathrm{D}}(\Omega))$$

Definition (Weak solution (Chen 2001))

Find $(s_{\mathrm{w}}, p_{\mathrm{w}})$ such that, with $s_{\mathrm{n}} := 1 - s_{\mathrm{w}}$,

$$s_{\mathrm{w}} \in C([0,T]; L^2(\Omega)),\ s_{\mathrm{w}}(\cdot, 0) = s^0_{\mathrm{w}},$$

$$\partial_t s_{\mathrm{w}} \in L^2((0,T); (H^1_{\mathrm{D}}(\Omega))'),$$

$$\mathfrak{p}(s_{\mathrm{w}}, p_{\mathrm{w}}) \in X,$$

$$\mathfrak{q}(s_{\mathrm{w}}) \in X,$$

$$\int_0^T \{\langle \partial_t(\phi s_\alpha), \varphi\rangle - (\mathbf{u}_\alpha(s_{\mathrm{w}}, p_{\mathrm{w}}), \nabla\varphi) - (q_\alpha, \varphi)\} \mathrm{d}t = 0$$

$$\forall \varphi \in X,\ \alpha \in \{\mathrm{n}, \mathrm{w}\}.$$

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Outline

Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau}) := \left\{ \sum_{\alpha\in\{{\rm n},{\rm w}\}} \left\{ \sup_{\varphi\in X|_{I_n},\, \|\varphi\|_{X|_{I_n}}=1} \int_{I_n} \{ \langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{u}_\alpha(s_{\rm w},p_{\rm w}) - \mathbf{u}_\alpha(s_{{\rm w},h\tau},p_{{\rm w},h\tau}), \nabla\varphi)\} {\rm d}t \right\}^2 \right\}^{\frac{1}{2}}$$

Theorem (Link energy-type error – dual norm of the residual)

Let $(s_{\rm w},p_{\rm w})$ be the weak solution. Let $(s_{{\rm w},h\tau},p_{{\rm w},h\tau})$ be arbitrary such that $\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\in X$ and $\mathfrak{q}(s_{{\rm w},h\tau})\in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\|s_{\rm w}-s_{{\rm w},h\tau}\|_{L^2((0,T);H^{-1}(\Omega))} + \|\mathfrak{q}(s_{\rm w})-\mathfrak{q}(s_{{\rm w},h\tau})\|_{L^2(\Omega\times(0,T))} + \|\mathfrak{p}(s_{\rm w},p_{\rm w})-\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\|_{L^2((0,T);H^1_0(\Omega))} \le C\left\{\sum_{n=1}^N \mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})^2\right\}^{\frac{1}{2}}$$

Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\mathrm{w}},p_{\mathrm{w}}}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}) := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \left\{ \sup_{\varphi\in X|_{I_n},\, \|\varphi\|_{X|_{I_n}}=1} \int_{I_n} \{\langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{u}_\alpha(s_{\mathrm{w}},p_{\mathrm{w}}) - \mathbf{u}_\alpha(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}), \nabla\varphi)\}\mathrm{d}t \right\}^2 \right\}^{\frac{1}{2}}$$

Theorem (Link energy-type error – dual norm of the residual)

Let $(s_{\mathrm{w}},p_{\mathrm{w}})$ be the weak solution. Let $(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau})$ be arbitrary such that $\mathfrak{p}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}) \in X$ and $\mathfrak{q}(s_{\mathrm{w},h\tau}) \in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\begin{aligned}&\|s_{\mathrm{w}} - s_{\mathrm{w},h\tau}\|_{L^2((0,T);H^{-1}(\Omega))} + \|\mathfrak{q}(s_{\mathrm{w}}) - \mathfrak{q}(s_{\mathrm{w},h\tau})\|_{L^2(\Omega\times(0,T))}\\ &+ \|\mathfrak{p}(s_{\mathrm{w}},p_{\mathrm{w}}) - \mathfrak{p}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau})\|_{L^2((0,T);H^1_0(\Omega))}\\ &\le C\left\{\sum_{n=1}^N \mathcal{J}^n_{s_{\mathrm{w}},p_{\mathrm{w}}}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau})^2\right\}^{\frac{1}{2}}\end{aligned}$$

Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau}) := \left\{ \sum_{\alpha\in\{{\rm n},{\rm w}\}} \left\{ \sup_{\varphi\in X|_{I_n},\, \|\varphi\|_{X|_{I_n}}=1} \int_{I_n} \{ \langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{u}_\alpha(s_{\rm w},p_{\rm w}) - \mathbf{u}_\alpha(s_{{\rm w},h\tau},p_{{\rm w},h\tau}), \nabla\varphi)\}{\rm d}t \right\}^2 \right\}^{\frac{1}{2}}$$

Theorem (Link energy-type error – dual norm of the residual)

Let $(s_{\rm w},p_{\rm w})$ be the weak solution. Let $(s_{{\rm w},h\tau},p_{{\rm w},h\tau})$ be arbitrary such that $\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\in X$ and $\mathfrak{q}(s_{{\rm w},h\tau})\in X$ (and satisfying the initial and boundary conditions for simplicity). Then

$$\|s_{\rm w}-s_{{\rm w},h\tau}\|_{L^2((0,T);H^{-1}(\Omega))} + \|\mathfrak{q}(s_{\rm w})-\mathfrak{q}(s_{{\rm w},h\tau})\|_{L^2(\Omega\times(0,T))} + \|\mathfrak{p}(s_{\rm w},p_{\rm w})-\mathfrak{p}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})\|_{L^2((0,T);H^1_0(\Omega))} \le C\left\{\sum_{n=1}^N \mathcal{J}^n_{s_{\rm w},p_{\rm w}}(s_{{\rm w},h\tau},p_{{\rm w},h\tau})^2\right\}^{\frac{1}{2}}$$

Link energy-type error – dual norm of the residual

Dual norm of the residual on the time interval I_n

$$\mathcal{J}^n_{s_{\mathrm{w}},p_{\mathrm{w}}}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}) := \left\{ \sum_{\alpha\in\{\mathrm{n},\mathrm{w}\}} \left\{ \sup_{\varphi\in X|_{I_n},\, \|\varphi\|_{X|_{I_n}}=1} \int_{I_n} \{ \langle \partial_t(\phi s_\alpha) - \partial_t(\phi s_{\alpha,h\tau}), \varphi\rangle - (\mathbf{u}_\alpha(s_{\mathrm{w}},p_{\mathrm{w}}) - \mathbf{u}_\alpha(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau}), \nabla\varphi)\}\,\mathrm{d}t \right\}^2 \right\}^{\frac{1}{2}}$$

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$$\|s_{\mathrm{w}} - s_{\mathrm{w},h\tau}\|_{L^2((0,T);H^{-1}(\Omega))} + \|\mathfrak{q}(s_{\mathrm{w}}) - \mathfrak{q}(s_{\mathrm{w},h\tau})\|_{L^2(\Omega\times(0,T))} + \|\mathfrak{p}(s_{\mathrm{w}},p_{\mathrm{w}}) - \mathfrak{p}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau})\|_{L^2((0,T);H^1_0(\Omega))} \le C\left\{\sum_{n=1}^N \mathcal{J}^n_{s_{\mathrm{w}},p_{\mathrm{w}}}(s_{\mathrm{w},h\tau},p_{\mathrm{w},h\tau})^2\right\}^{\frac{1}{2}}$$

Distinguishing the error components

Theorem (Distinguishing the error components)

Consider a vertex-centered finite volume / backward Euler approximation. Let

- n *be the time step,*
- k *be the linearization step,*
- i *be the algebraic solver step,*

with the approximations $(s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w},h\tau}^{n,k,i})$*. Then*

$$\mathcal{J}_{s_\mathrm{w},p_\mathrm{w}}^{n}(s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w},h\tau}^{n,k,i}) \leq \eta_{\mathrm{sp}}^{n,k,i} + \eta_{\mathrm{tm}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}.$$

Error components

- $\eta_{\mathrm{sp}}^{n,k,i}$: spatial discretization
- $\eta_{\mathrm{tm}}^{n,k,i}$: temporal discretization
- $\eta_{\mathrm{lin}}^{n,k,i}$: linearization
- $\eta_{\mathrm{alg}}^{n,k,i}$: algebraic solver

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$$\mathcal{J}^n_{s_{\mathrm{w}},p_{\mathrm{w}}}(s_{\mathrm{w},h\tau}^{n,k,i}, p_{\mathrm{w},h\tau}^{n,k,i}) \leq \eta_{\mathrm{sp}}^{n,k,i} + \eta_{\mathrm{tm}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}.$$

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Outline

Iteratively coupled vertex-centered finite volumes

Vertex-centered finite volumes

- simplicial meshes $\mathcal{T}_h^n$, dual meshes $\mathcal{D}_h^n$
- discrete saturations and pressures continuous and piecewise affine on $\mathcal{T}_h^n$

Implicit pressure equation on step k

$$-\left(\left(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\right)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k}\cdot\mathbf{n}_D \right.$$
$$\left. +\lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D, 1\right)_{\partial D\setminus\partial\Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$

Explicit saturation equation on step k

$$s_{\mathrm{w},D}^{n,k} := \frac{\tau^n}{\phi|D|}\left(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k}\cdot\mathbf{n}_D, 1\right)_{\partial D\setminus\partial\Omega} + s_{\mathrm{w},D}^{n-1} \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$

Iteratively coupled vertex-centered finite volumes

Vertex-centered finite volumes

- simplicial meshes $\mathcal{T}_h^n$, dual meshes $\mathcal{D}_h^n$
- discrete saturations and pressures continuous and piecewise affine on $\mathcal{T}_h^n$

Implicit pressure equation on step k

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Iteratively coupled vertex-centered finite volumes

Vertex-centered finite volumes

- simplicial meshes $\mathcal{T}_h^n$, dual meshes $\mathcal{D}_h^n$
- discrete saturations and pressures continuous and piecewise affine on $\mathcal{T}_h^n$

Implicit pressure equation on step k

$$-\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla \overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D, 1\Big)_{\partial D\setminus\partial\Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$

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Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$-\left(\left(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\right)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D, 1\right)_{\partial D\setminus\partial\Omega} = -R_{\mathrm{t},D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$

$$s_{\mathrm{w},D}^{n,k,i} := \frac{\tau^n}{\phi|D|}\left(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D, 1\right)_{\partial D\setminus\partial\Omega} + s_{\mathrm{w},D}^{n-1}$$

Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$-\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D, 1\Big)_{\partial D\setminus\partial\Omega} = -R_{\mathrm{t},D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\mathrm{int},n}$$

$$s_{\mathrm{w},D}^{n,k,i} := \frac{\tau^n}{\phi|D|}\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D, 1\big)_{\partial D\setminus\partial\Omega} + s_{\mathrm{w},D}^{n-1}$$

Velocities reconstructions

Total phase velocities reconstructions

$$(\mathbf{d}_{\mathrm{t},h}^{n,k,i}\cdot\mathbf{n}_D,1)_e := -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i})+\lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D,1\Big)_e,$$

$$((\mathbf{d}_{\mathrm{t},h}^{n,k,i}+\mathbf{l}_{\mathrm{t},h}^{n,k,i})\cdot\mathbf{n}_D,1)_e := -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})+\lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D,1\Big)_e,$$

$$\mathbf{a}_{\mathrm{t},h}^{n,k,i} := \mathbf{d}_{\mathrm{t},h}^{n,k,i+\nu}+\mathbf{l}_{\mathrm{t},h}^{n,k,i+\nu}-(\mathbf{d}_{\mathrm{t},h}^{n,k,i}+\mathbf{l}_{\mathrm{t},h}^{n,k,i})$$

Wetting phase velocities reconstructions

$$(\mathbf{d}_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1)_e := -\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1\big)_e,$$

$$((\mathbf{d}_{\mathrm{w},h}^{n,k,i}+\mathbf{l}_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D,1)_e := -\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1\big)_e,$$

$$\mathbf{a}_{\mathrm{w},h}^{n,k,i} := 0$$

Nonwetting phase and total velocities reconstructions

- $\mathbf{d}_{\mathrm{n},h}^{n,k,i}:=\mathbf{d}_{\mathrm{t},h}^{n,k,i}-\mathbf{d}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{l}_{\mathrm{n},h}^{n,k,i}:=\mathbf{l}_{\mathrm{t},h}^{n,k,i}-\mathbf{l}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{a}_{\mathrm{n},h}^{n,k,i}:=\mathbf{a}_{\mathrm{t},h}^{n,k,i}-\mathbf{a}_{\mathrm{w},h}^{n,k,i}$
- $\mathbf{t}_{\cdot,h}^{n,k,i} := \mathbf{d}_{\cdot,h}^{n,k,i}+\mathbf{l}_{\cdot,h}^{n,k,i}+\mathbf{a}_{\cdot,h}^{n,k,i}$

Velocities reconstructions

Total phase velocities reconstructions

$$(\mathbf{d}_{\mathrm{t},h}^{n,k,i}\cdot\mathbf{n}_D,1)_e := -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i})+\lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D,1\Big)_e,$$

$$((\mathbf{d}_{\mathrm{t},h}^{n,k,i}+\mathbf{l}_{\mathrm{t},h}^{n,k,i})\cdot\mathbf{n}_D,1)_e := -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})+\lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\overline{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D,1\Big)_e,$$

$$\mathbf{a}_{\mathrm{t},h}^{n,k,i} := \mathbf{d}_{\mathrm{t},h}^{n,k,i+\nu}+\mathbf{l}_{\mathrm{t},h}^{n,k,i+\nu}-(\mathbf{d}_{\mathrm{t},h}^{n,k,i}+\mathbf{l}_{\mathrm{t},h}^{n,k,i})$$

Wetting phase velocities reconstructions

$$(\mathbf{d}_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1)_e := -\Big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1\Big)_e,$$

$$((\mathbf{d}_{\mathrm{w},h}^{n,k,i}+\mathbf{l}_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D,1)_e := -\Big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D,1\Big)_e,$$

$$\mathbf{a}_{\mathrm{w},h}^{n,k,i} := 0$$

Nonwetting phase and total velocities reconstructions

- $\mathbf{d}_{\mathrm{n},h}^{n,k,i}:=\mathbf{d}_{\mathrm{t},h}^{n,k,i}-\mathbf{d}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{l}_{\mathrm{n},h}^{n,k,i}:=\mathbf{l}_{\mathrm{t},h}^{n,k,i}-\mathbf{l}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{a}_{\mathrm{n},h}^{n,k,i}:=\mathbf{a}_{\mathrm{t},h}^{n,k,i}-\mathbf{a}_{\mathrm{w},h}^{n,k,i}$
- $\mathbf{t}_{\cdot,h}^{n,k,i}:=\mathbf{d}_{\cdot,h}^{n,k,i}+\mathbf{l}_{\cdot,h}^{n,k,i}+\mathbf{a}_{\cdot,h}^{n,k,i}$

Velocities reconstructions

Total phase velocities reconstructions

$$
\begin{aligned}
(\mathbf{d}_{\mathrm{t},h}^{n,k,i}\cdot\mathbf{n}_D, 1)_e := & -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D \\
& + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla\bar{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D, 1\Big)_e, \\
((\mathbf{d}_{\mathrm{t},h}^{n,k,i} + \mathbf{l}_{\mathrm{t},h}^{n,k,i})\cdot\mathbf{n}_D, 1)_e := & -\Big(\big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1}) + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\big)\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D \\
& + \lambda_{\mathrm{r,n}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla\bar{p}_{\mathrm{c}}(s_{\mathrm{w},h}^{n,k-1})\cdot\mathbf{n}_D, 1\Big)_e, \\
\mathbf{a}_{\mathrm{t},h}^{n,k,i} := & \ \mathbf{d}_{\mathrm{t},h}^{n,k,i+\nu} + \mathbf{l}_{\mathrm{t},h}^{n,k,i+\nu} - (\mathbf{d}_{\mathrm{t},h}^{n,k,i} + \mathbf{l}_{\mathrm{t},h}^{n,k,i})
\end{aligned}
$$

Wetting phase velocities reconstructions

$$
\begin{aligned}
(\mathbf{d}_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D, 1)_e := & -\Big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k,i})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D, 1\Big)_e, \\
((\mathbf{d}_{\mathrm{w},h}^{n,k,i} + \mathbf{l}_{\mathrm{w},h}^{n,k,i})\cdot\mathbf{n}_D, 1)_e := & -\Big(\lambda_{\mathrm{r,w}}(s_{\mathrm{w},h}^{n,k-1})\underline{\mathbf{K}}\nabla p_{\mathrm{w},h}^{n,k,i}\cdot\mathbf{n}_D, 1\Big)_e, \\
\mathbf{a}_{\mathrm{w},h}^{n,k,i} := & \ 0
\end{aligned}
$$

Nonwetting phase and total velocities reconstructions

- $\mathbf{d}_{\mathrm{n},h}^{n,k,i} := \mathbf{d}_{\mathrm{t},h}^{n,k,i} - \mathbf{d}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{l}_{\mathrm{n},h}^{n,k,i} := \mathbf{l}_{\mathrm{t},h}^{n,k,i} - \mathbf{l}_{\mathrm{w},h}^{n,k,i}$, $\mathbf{a}_{\mathrm{n},h}^{n,k,i} := \mathbf{a}_{\mathrm{t},h}^{n,k,i} - \mathbf{a}_{\mathrm{w},h}^{n,k,i}$
- $\mathbf{t}_{\cdot,h}^{n,k,i} := \mathbf{d}_{\cdot,h}^{n,k,i} + \mathbf{l}_{\cdot,h}^{n,k,i} + \mathbf{a}_{\cdot,h}^{n,k,i}$

Model problem

Horizontal flow

$$\partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\underline{\mathbf{K}}\nabla p_\alpha\right) = 0,$$

$$s_\mathrm{n} + s_\mathrm{w} = 1,$$

$$p_\mathrm{n} - p_\mathrm{w} = p_\mathrm{c}(s_\mathrm{w})$$

Brooks–Corey model

- relative permeabilities

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

- capillary pressure

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

-

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

Model problem

Horizontal flow

$$\partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\underline{\mathbf{K}}\nabla p_\alpha\right) = 0,$$

$$s_\mathrm{n} + s_\mathrm{w} = 1,$$

$$p_\mathrm{n} - p_\mathrm{w} = p_\mathrm{c}(s_\mathrm{w})$$

Brooks–Corey model

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

- capillary pressure

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

-

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

Data from Klieber & Rivière (2006)

Data

$$\Omega = (0,300)\mathrm{m} \times (0,300)\mathrm{m}, \quad T = 4{\cdot}10^6\mathrm{s},$$
$$\phi = 0.2, \quad \underline{\mathbf{K}} = 10^{-11}\underline{\mathbf{I}}\,\mathrm{m}^2,$$
$$\mu_{\rm w} = 5{\cdot}10^{-4}\mathrm{kg\,m^{-1}s^{-1}}, \quad \mu_{\rm n} = 2{\cdot}10^{-3}\mathrm{kg\,m^{-1}s^{-1}},$$
$$s_{\rm rw} = s_{\rm rn} = 0, \quad p_{\rm d} = 5{\cdot}10^3\mathrm{kg\,m^{-1}s^{-2}}$$

Initial condition ($\widetilde{K}$ 18m × 18m lower left corner block)

$$s_{\rm w}^0 = 0.2 \text{ on } K \in \mathcal{T}_h,\ K \notin \widetilde{K},$$
$$s_{\rm w}^0 = 0.95 \text{ on } K \in \mathcal{T}_h,\ K \in \widetilde{K}$$

Boundary conditions ($\widehat{K}$ 18m × 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial\widetilde{K} \cap \partial\Omega$ and $\partial\widehat{K} \cap \partial\Omega$
- $\widetilde{K}$ – injection well: $s_{\rm w} = 0.95$, $p_{\rm w} = 3.45{\cdot}10^6\mathrm{kg\,m^{-1}s^{-2}}$
- $\widehat{K}$ – production well: $s_{\rm w} = 0.2$, $p_{\rm w} = 2.41{\cdot}10^6\mathrm{kg\,m^{-1}s^{-2}}$

Data from Klieber & Rivière (2006)

Data

$$\Omega = (0,300)\mathrm{m} \times (0,300)\mathrm{m}, \quad T = 4{\cdot}10^6\mathrm{s},$$
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Initial condition ($\widetilde{K}$ 18m × 18m lower left corner block)

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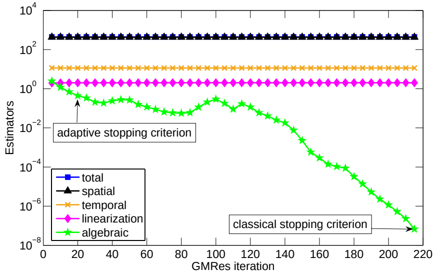
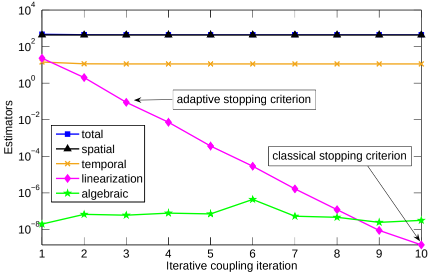
Estimators and stopping criteria

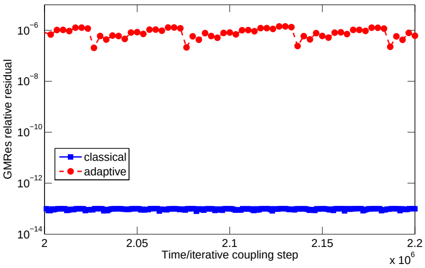


Estimators in function of GMRes iterations

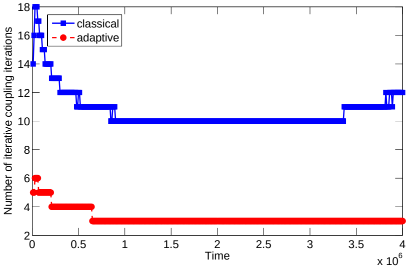


Estimators in function of iterative coupling iterations

GMRes relative residual/iterative coupling iterations

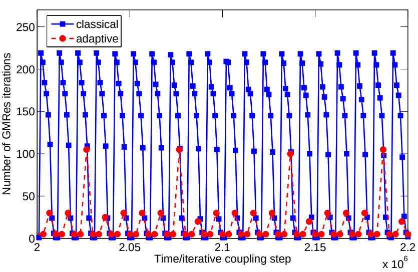


GMRes relative residual

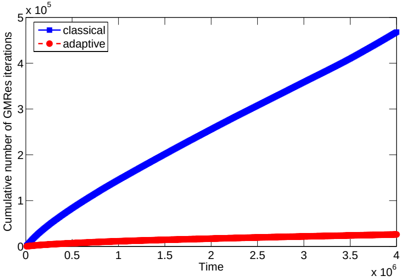


Iterative coupling iterations

GMRes iterations

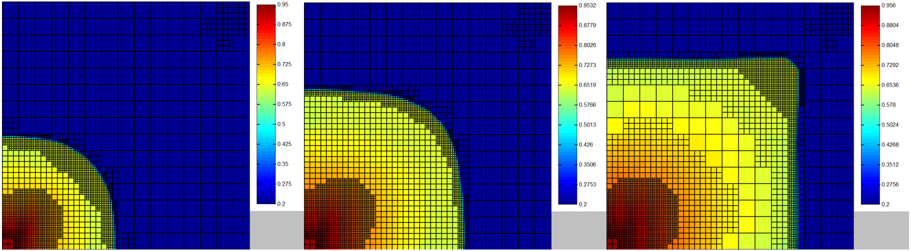


Per time and iterative coupling step



Cumulated

Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

Outline

Multiphase compositional flows

Governing partial differential equations

- conservation of mass for components

$$\partial_t l_c + \nabla \cdot \mathbf{\Phi}_c = q_c, \qquad \forall c \in \mathcal{C}$$

- + boundary & initial conditions

Constitutive laws

- phase pressures – reference pressure – capillary pressure

$$P_p := P + P_{c_p}(\boldsymbol{S})$$

- Darcy's law

$$\mathbf{u}_p(P_p, \boldsymbol{C}_p) := -\underline{\mathbf{K}}\,(\nabla P_p + \rho_p(P_p, \boldsymbol{C}_p) g \nabla z)$$

- component fluxes

$$\Phi_c := \sum_{p \in \mathcal{P}_c} \Phi_{p,c}, \qquad \Phi_{p,c} := \nu_p(P_p, \boldsymbol{S}, \boldsymbol{C}_p) C_{p,c} \mathbf{u}_p(P_p, \boldsymbol{C}_p)$$

- amount of moles of component c per unit volume

$$l_c := \phi \sum_{p \in \mathcal{P}_c} \zeta_p(P_p, \boldsymbol{C}_p) S_p C_{p,c}$$

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Multiphase compositional flows

Closure algebraic equations

- conservation of pore volume: $\sum_{p\in\mathcal{P}} S_p = 1$
- conservation of the quantity of the matter: $\sum_{c\in\mathcal{C}_p} C_{p,c} = 1$ for all $p \in \mathcal{P}$
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- coupled system
- unsteady, nonlinear
- elliptic–parabolic degenerate type
- dominant advection

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Outline

Weak solution

Energy spaces

$$X := L^2((0,T); H^1(\Omega)),$$
$$Y := H^1((0,T); L^2(\Omega))$$

Definition (Weak solution)

Find $(P, (S_p)_{p\in\mathcal{P}}, (C_{p,c})_{p\in\mathcal{P}, c\in\mathcal{C}_p}$ such that

$$l_c \in Y \qquad \forall c \in \mathcal{C},$$
$$P_p(P, \boldsymbol{S}) \in X \qquad \forall p \in \mathcal{P},$$
$$\Phi_c \in [L^2((0,T); L^2(\Omega))]^d \qquad \forall c \in \mathcal{C},$$
$$\int_0^T \{(\partial_t l_c, \varphi)(t) - (\Phi_c, \nabla\varphi)(t)\}\,\mathrm{d}t = \int_0^T (q_c, \varphi)(t)\mathrm{d}t \quad \forall \varphi \in X, \forall c \in \mathcal{C},$$

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Fully implicit cell-centered finite volume scheme

Fully implicit cell-centered finite volumes

Time step n, Newton iteration k, and linear solver iteration i: find $\mathcal{X}_K^{n,k,i} := (P_K^{n,k,i}, (S_{p,K}^{n,k,i})_{p\in\mathcal{P}}, (C_{p,c,K}^{n,k,i})_{p\in\mathcal{P},c\in\mathcal{C}_p}, K \in \mathcal{T}_h^n$, s. t.

$$\frac{|K|}{\tau^n}\left(l_{c,K}(\mathcal{X}_h^{n,k-1}) + \mathcal{L}_{c,K}^{n,k,i} - l_{c,K}^{n-1}\right) + \sum_{e\in\mathcal{E}_K^{\mathrm{int},n}} F_{c,M,e}^{n,k,i} - |K|q_{c,K}^n$$

$$= R_{c,K}^{n,k,i} \qquad \forall c \in \mathcal{C},\ \forall K \in \mathcal{T}_h^n,$$

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Estimate distinguishing different error components

Theorem (Estimate distinguishing different error components)

Consider

- *time step n,*
- *linearization step k,*
- *iterative algebraic solver step i,*

and the corresponding approximations. Then

$$(\textit{dual error + nonconformity})_{I_n} \leq \eta_{\mathrm{sp}}^{n,k,i} + \eta_{\mathrm{tm}}^{n,k,i} + \eta_{\mathrm{lin}}^{n,k,i} + \eta_{\mathrm{alg}}^{n,k,i}.$$

Error components

- $\eta_{\mathrm{sp}}^{n,k,i}$: spatial discretization
- $\eta_{\mathrm{tm}}^{n,k,i}$: temporal discretization
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Outline

Test case and numerical setting

Test case

- two-spot setting
- two phases and three components
- homogeneous/heterogeneous permeability distribution

Discretization and resolution

- fully implicit cell-centered finite volumes
- Newton linearization
- GMRes with ILU0 preconditioning algebraic solver

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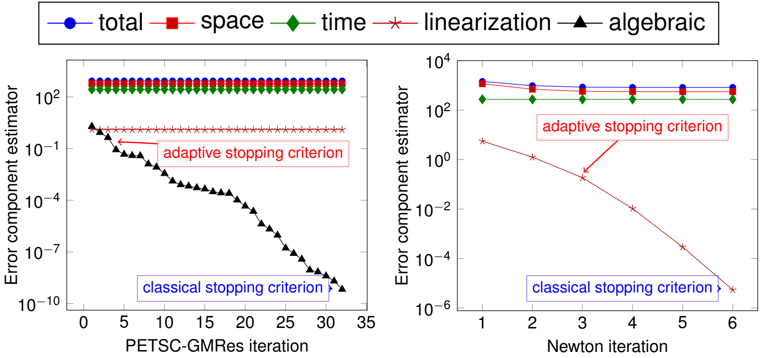
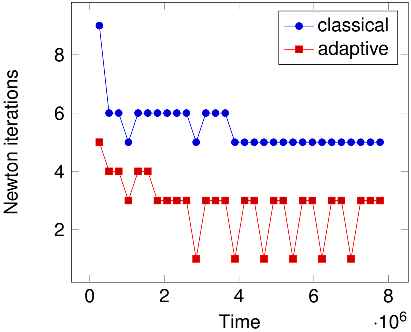


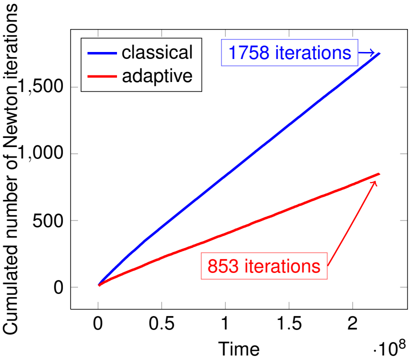
Estimators w.r.t. GMRes iterations

Estimators w.r.t. Newton iterations

Newton iterations

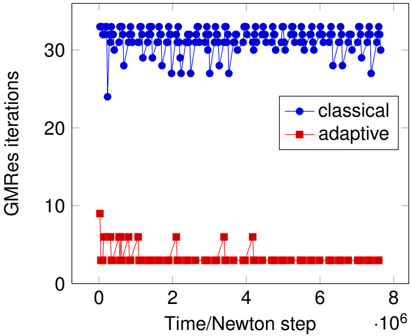


Per time step

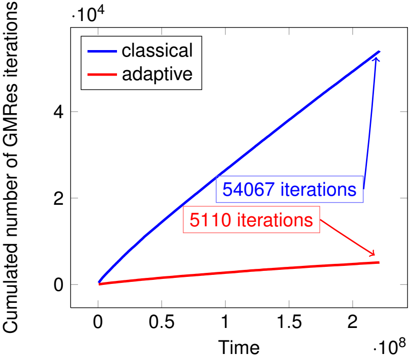


Cumulated

GMRes iterations



Per time and Newton step



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Outline

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Entire adaptivity

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- **"online decisions"**: algebraic step / linearization step / space mesh refinement / time step modification
- important **computational savings**
- guaranteed and robust **a posteriori error estimates**

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- other coupled nonlinear systems
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Thank you for your attention!