

A posteriori control of numerical error
and stopping criteria
for linear and nonlinear solvers

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Paris, May 16, 2013

Outline

- 1 Introduction
- 2 Adaptive inexact Newton method
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Numerical results
- 3 Application to two-phase flow in porous media
 - A guaranteed a posteriori error estimate
 - Fully implicit cell-centered finite volumes
 - Iteratively coupled implicit pressure–explicit saturation vertex-centered finite volumes
- 4 Conclusions and future directions

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Inexact Newton method

System of nonlinear algebraic equations

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

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

Algorithm (Inexact 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.)

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

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
- Deuffhard (1990's), adaptive damping and multigrid

Stopping criteria for algebraic solvers

- engineering literature, since 1950's
- Becker, Johnson, and Rannacher (1995), multigrid

A posteriori error estimates for nonlinear problems

- Han (1994), general framework
- Verfürth (1994), residual estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors

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Quasi-linear elliptic problem

Quasi-linear elliptic problem

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

Example

p -Laplacian: $\sigma(u, \nabla u) = |\nabla u|^{p-2} \nabla u$, $p \in (1, +\infty)$

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

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

Weak formulation

Find $u \in V$ such that

$$A(u) = f \text{ in } V'$$

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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A posteriori error estimate

Assumption A (Total flux reconstruction)

There exists a *flux reconstruction* $\mathbf{t}_h^{k,i} \in \mathbf{H}^q(\text{div}, \Omega)$ such that

$$\nabla \cdot \mathbf{t}_h^{k,i} \approx f.$$

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

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

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

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Estimate distinguishing error components

Theorem (Estimate distinguishing different error components)

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

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Stopping criteria

Global stopping criteria

- stop whenever:

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

$$\eta_{\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i}$$

- $\gamma_{\text{alg}}, \gamma_{\text{lin}} \approx 0.1$

Local stopping criteria

- stop whenever:

$$\eta_{\text{alg},K}^{k,i} \leq \gamma_{\text{alg},K} \max \{ \eta_{\text{disc},K}^{k,i}, \eta_{\text{lin},K}^{k,i} \} \quad \forall K \in \mathcal{T}_h,$$

$$\eta_{\text{lin},K}^{k,i} \leq \gamma_{\text{lin},K} \eta_{\text{disc},K}^{k,i} \quad \forall K \in \mathcal{T}_h$$

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- $\gamma_{\text{alg},K}, \gamma_{\text{lin},K} \approx 0.1$

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,

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

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

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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$$\begin{aligned} & \eta_{\text{disc},K}^{k,i} + \eta_{\text{lin},K}^{k,i} + \eta_{\text{alg},K}^{k,i} \\ & \lesssim \mathcal{J}_{u,\mathfrak{T}_K}^{\text{up}}(u_h^{k,i}) + \eta_{\text{quad},\mathfrak{T}_K}^{k,i} + \eta_{\text{osc},\mathfrak{T}_K}^{k,i} \end{aligned}$$

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- **robustness** and **local efficiency** for an upper bound on the dual norm

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Numerical experiment I

Model problem

- p -Laplacian

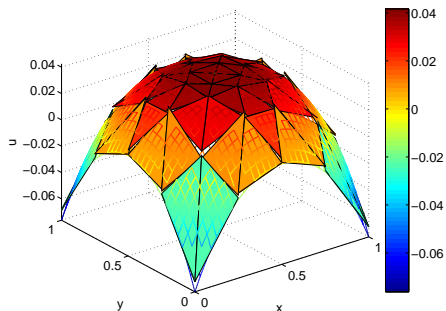
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

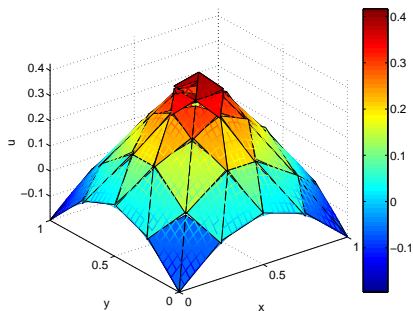
$$u(x, y) = -\frac{p-1}{p} \left((x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left(\frac{1}{2} \right)^{\frac{p}{p-1}}$$

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

Analytical and approximate solutions

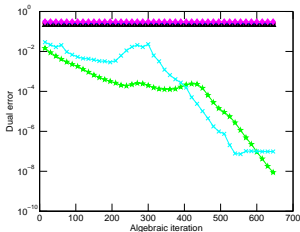


Case $p = 1.5$

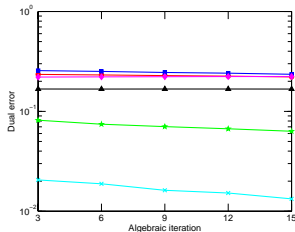


Case $p = 10$

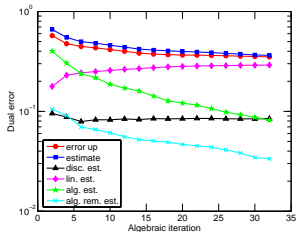
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

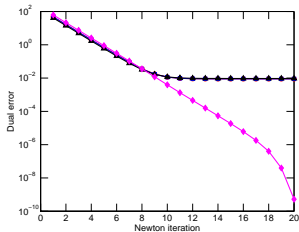


inexact Newton

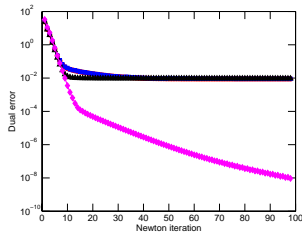


ad. inexact Newton

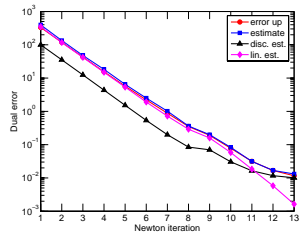
Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh



Newton

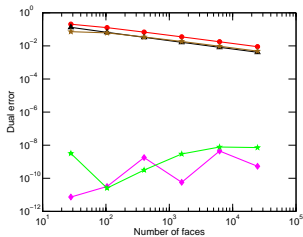


inexact Newton

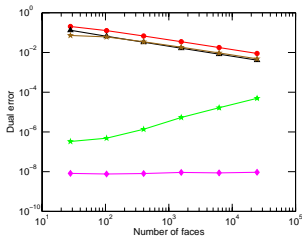


ad. inexact Newton

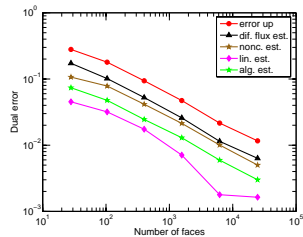
Error and estimators, $p = 10$



Newton

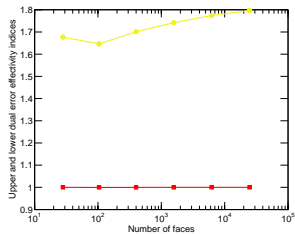


inexact Newton

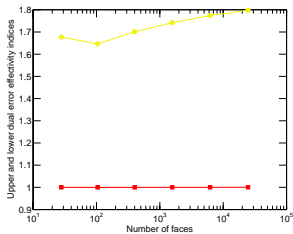


ad. inexact Newton

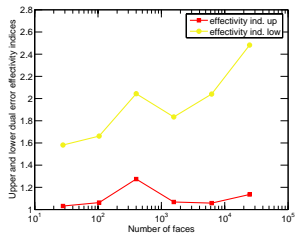
Effectivity indices, $p = 10$



Newton

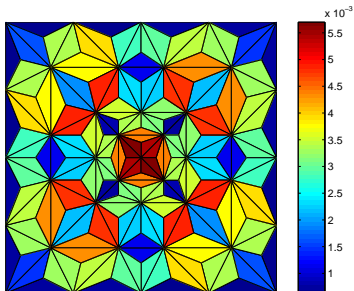


inexact Newton

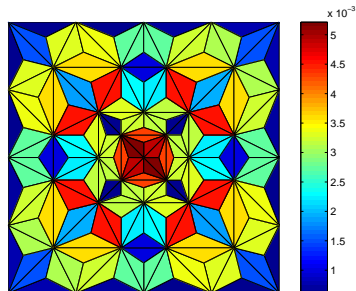


ad. inexact Newton

Error distribution, $p = 10$

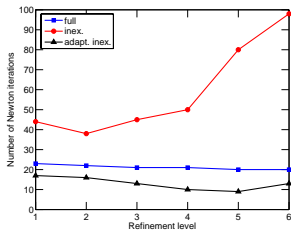


Estimated error distribution

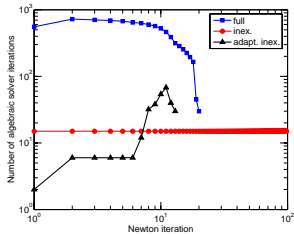


Exact error distribution

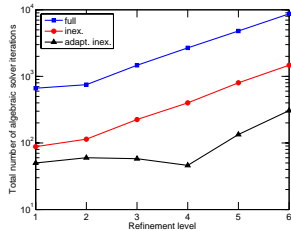
Newton and algebraic iterations, $p = 10$



Newton it. / refinement

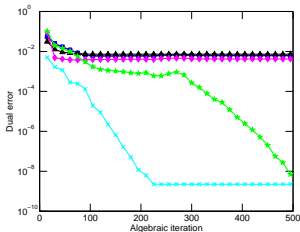


alg. it. / Newton step

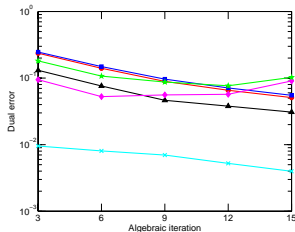


alg. it. / refinement

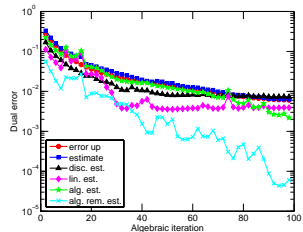
Error and estimators as a function of CG iterations, $\rho = 1.5$, 6th level mesh, 1st Newton step.



Newton

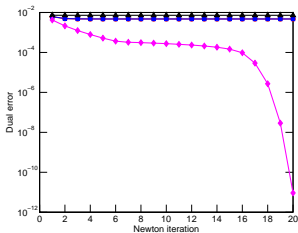


inexact Newton

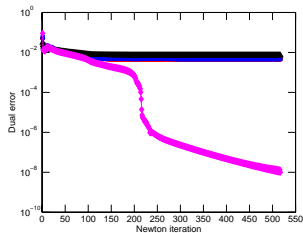


ad. inexact Newton

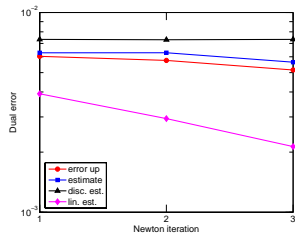
Error and estimators as a function of Newton iterations, $p = 1.5$, 6th level mesh



Newton

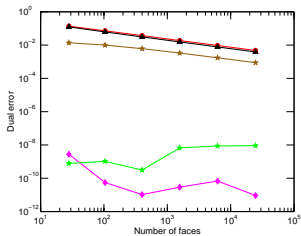


inexact Newton

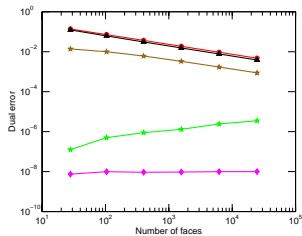


ad. inexact Newton

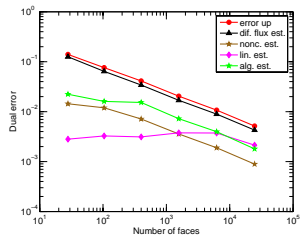
Error and estimators, $p = 1.5$



Newton

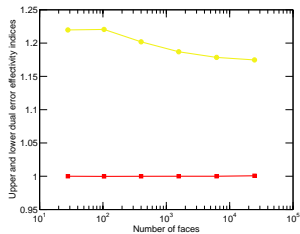


inexact Newton

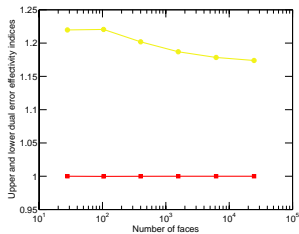


ad. inexact Newton

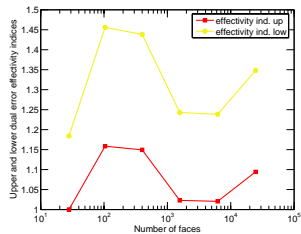
Effectivity indices, $p = 1.5$



Newton

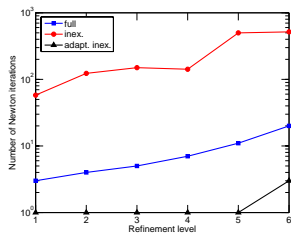


inexact Newton

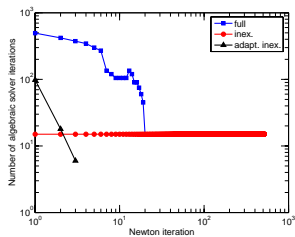


ad. inexact Newton

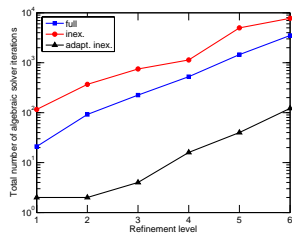
Newton and algebraic iterations, $p = 1.5$



Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p -Laplacian

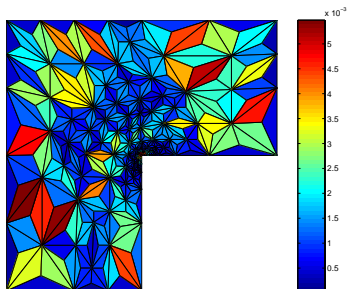
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

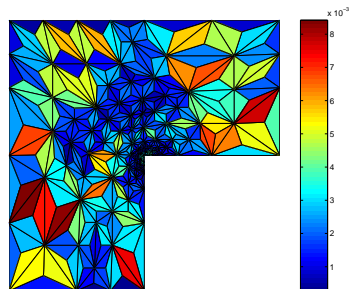
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

Error distribution on an adaptively refined mesh

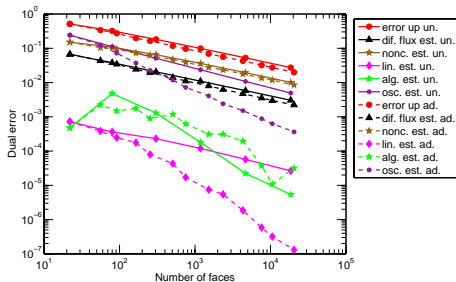


Estimated error distribution

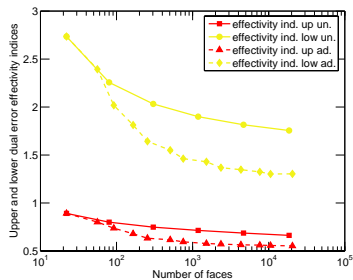


Exact error distribution

Estimated and actual errors and the effectivity index

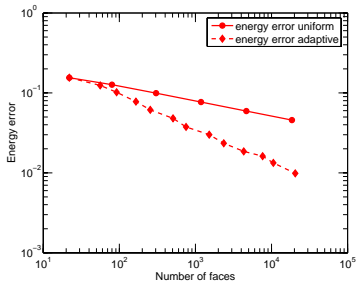


Estimated and actual errors

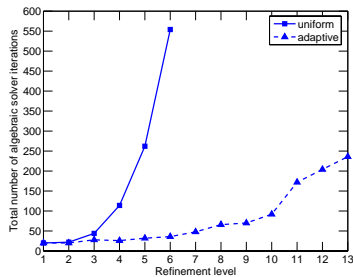


Effectivity index

Energy error and overall performance



Energy error



Overall performance

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Two-phase flow

Horizontal two-phase flow in porous media

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

$$s_n + s_w = 1,$$

$$p_n - p_w = \pi(s_w)$$

Mathematical issues

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

Brooks–Corey model, $s_e := \frac{s_w - s_{rw}}{1 - s_{rw} - s_{rn}}$

- relative permeabilities

$$k_{r,w}(s_w) = s_e^4, \quad k_{r,n}(s_w) = (1 - s_e)^2(1 - s_e^2)$$

- capillary pressure

$$\pi(s_w) = p_d s_e^{-\frac{1}{2}}$$

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Two-phase flow in porous media

Theorem (A posteriori error estimate distinguishing the error components)

Let

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

with the approximations $(s_{w,h_T}^{n,k,i}, p_{w,h_T}^{n,k,i})$. Then

$$\| (s_w - s_{w,h_T}^{n,k,i}, p_w - p_{w,h_T}^{n,k,i}) \|_I \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}.$$

Error components

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

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Error components

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

Local estimators

- *spatial estimators*

$$\eta_{\text{sp},K}^{n,k,i}(t) := \left\{ \begin{aligned} & \sum_{\alpha \in \{\text{n,w}\}} (\|\mathbf{d}_{\alpha,h}^{n,k,i} - \mathbf{v}_{\alpha}(p_{w,h}^{n,k,i}, \mathbf{s}_{w,h}^{n,k,i})\|_K \\ & + h_K/\pi \|q_{\alpha}^n - \partial_t^n(\phi \mathbf{s}_{\alpha,h\tau}^{n,k,i}) - \nabla \cdot \mathbf{u}_{\alpha,h}^{n,k,i}\|_K)^2 \\ & + (\|\underline{\mathbf{K}}(\lambda_w(\mathbf{s}_{w,h\tau}^{n,k,i}) + \lambda_n(\mathbf{s}_{w,h\tau}^{n,k,i}))\nabla(p(p_{w,h\tau}^{n,k,i}, \mathbf{s}_{w,h\tau}^{n,k,i}) - \bar{p}_{h\tau}^{n,k,i})\|_K(t))^2 \\ & + (\|\underline{\mathbf{K}}\nabla(q(\mathbf{s}_{w,h\tau}^{n,k,i}) - \bar{q}_{h\tau}^{n,k,i})\|_K(t))^2 \end{aligned} \right\}^{\frac{1}{2}}$$

- *temporal estimators*

$$\eta_{\text{tm},K,\alpha}^{n,k,i}(t) := \|\mathbf{v}_{\alpha}(p_{w,h\tau}^{n,k,i}, \mathbf{s}_{w,h\tau}^{n,k,i})(t) - \mathbf{v}_{\alpha}(p_{w,h\tau}^{n,k,i}, \mathbf{s}_{w,h\tau}^{n,k,i})(t^n)\|_K \quad \alpha \in \{\text{n,w}\}$$

- *linearization estimators*

$$\eta_{\text{lin},K,\alpha}^{n,k,i} := \|\mathbf{l}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\text{n,w}\}$$

- *algebraic estimators*

$$\eta_{\text{alg},K,\alpha}^{n,k,i} := \|\mathbf{a}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\text{n,w}\}$$

Global estimators

Global estimators

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

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

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

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

Quarter five spot test problem

Data from Klieber & Rivière (2006)

$$\Omega = (0, 300)\text{m} \times (0, 300)\text{m}, \quad T = 4 \cdot 10^6 \text{s},$$

$$\phi = 0.2, \quad \underline{\mathbf{K}} = 10^{-11} \underline{\mathbf{I}} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial \tilde{K} \cap \partial \Omega$ and $\partial \hat{K} \cap \partial \Omega$

- \tilde{K} – injection well: $s_w = 0.95$, $\rho_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

- \hat{K} – production well: $s_w = 0.2$, $\rho_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

Quarter five spot test problem

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$$\phi = 0.2, \quad \mathbf{K} = 10^{-11} \mathbf{I} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial \tilde{K} \cap \partial \Omega$ and $\partial \hat{K} \cap \partial \Omega$

- \tilde{K} – injection well: $s_w = 0.95$, $\rho_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

- \hat{K} – production well: $s_w = 0.2$, $\rho_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

Quarter five spot test problem

Data from Klieber & Rivière (2006)

$$\Omega = (0, 300)\text{m} \times (0, 300)\text{m}, \quad T = 4 \cdot 10^6 \text{s},$$

$$\phi = 0.2, \quad \mathbf{K} = 10^{-11} \mathbf{I} \text{m}^2,$$

$$\mu_w = 5 \cdot 10^{-4} \text{kg m}^{-1} \text{s}^{-1}, \quad \mu_n = 2 \cdot 10^{-3} \text{kg m}^{-1} \text{s}^{-1},$$

$$s_{rw} = s_{rn} = 0, \quad \rho_d = 5 \cdot 10^3 \text{kg m}^{-1} \text{s}^{-2}$$

Initial condition (\tilde{K} 18m \times 18m lower left corner block)

$$s_w^0 = 0.2 \text{ on } K \in \mathcal{T}_h, K \notin \tilde{K},$$

$$s_w^0 = 0.95 \text{ on } K \in \mathcal{T}_h, K \in \tilde{K}$$

Boundary conditions (\hat{K} 18m \times 18m upper right corner block)

- no flow Neumann boundary conditions everywhere except of $\partial\tilde{K} \cap \partial\Omega$ and $\partial\hat{K} \cap \partial\Omega$
- \tilde{K} – injection well: $s_w = 0.95$, $\rho_w = 3.45 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$
- \hat{K} – production well: $s_w = 0.2$, $\rho_w = 2.41 \cdot 10^6 \text{kg m}^{-1} \text{s}^{-2}$

Outline

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- 2 Adaptive inexact Newton method
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Numerical results
- 3 Application to two-phase flow in porous media
 - A guaranteed a posteriori error estimate
 - **Fully implicit cell-centered finite volumes**
 - Iteratively coupled implicit pressure–explicit saturation vertex-centered finite volumes
- 4 Conclusions and future directions

Cell-centered finite volume scheme

Cell-centered finite volume scheme

For all $1 \leq n \leq N$, look for $s_{w,h}^n, \bar{p}_{w,h}^n$ such that

$$\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,\sigma_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

$$-\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,\sigma_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

where the fluxes are given by

$$F_{w,\sigma_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\eta_{r,w}(s_{w,K}^n) + \eta_{r,w}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \frac{\bar{p}_{w,L}^n - \bar{p}_{w,K}^n}{|\mathbf{x}_K - \mathbf{x}_L|} |\sigma_{KL}|,$$

$$F_{n,\sigma_{KL}}(s_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\eta_{r,n}(s_{w,K}^n) + \eta_{r,n}(s_{w,L}^n)}{2} |\underline{\mathbf{K}}| \\ \times \frac{\bar{p}_{w,L}^n + \pi(s_{w,L}^n) - (\bar{p}_{w,K}^n + \pi(s_{w,K}^n))}{|\mathbf{x}_K - \mathbf{x}_L|}$$

Cell-centered finite volume scheme

Cell-centered finite volume scheme

For all $1 \leq n \leq N$, look for $\mathbf{s}_{w,h}^n, \bar{p}_{w,h}^n$ such that

$$\phi \frac{\mathbf{s}_{w,K}^n - \mathbf{s}_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,\sigma_{KL}}(\mathbf{s}_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

$$-\phi \frac{\mathbf{s}_{w,K}^n - \mathbf{s}_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,\sigma_{KL}}(\mathbf{s}_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

where the fluxes are given by

$$F_{w,\sigma_{KL}}(\mathbf{s}_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\eta_{r,w}(\mathbf{s}_{w,K}^n) + \eta_{r,w}(\mathbf{s}_{w,L}^n)}{2} |\underline{\mathbf{K}}| \frac{\bar{p}_{w,L}^n - \bar{p}_{w,K}^n}{|\mathbf{x}_K - \mathbf{x}_L|} |\sigma_{KL}|,$$

$$F_{n,\sigma_{KL}}(\mathbf{s}_{w,h}^n, \bar{p}_{w,h}^n) := - \frac{\eta_{r,n}(\mathbf{s}_{w,K}^n) + \eta_{r,n}(\mathbf{s}_{w,L}^n)}{2} |\underline{\mathbf{K}}| \\ \times \frac{\bar{p}_{w,L}^n + \pi(\mathbf{s}_{w,L}^n) - (\bar{p}_{w,K}^n + \pi(\mathbf{s}_{w,K}^n))}{|\mathbf{x}_K - \mathbf{x}_L|}$$

Linearization and algebraic solution

Linearization step k and algebraic step i

Couple $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$ such that

$$\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$$

$$-\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$$

where the linearized fluxes are given by

$$\begin{aligned} F_{\alpha,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) &:= F_{\alpha,\sigma_{KL}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,\sigma_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,\sigma_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}). \end{aligned}$$

Linearization and algebraic solution

Linearization step k and algebraic step i

Couple $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$ such that

$$\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{w,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$$

$$-\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{\sigma_{KL} \in \mathcal{E}_K^{\text{int}}} F_{n,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$$

where the linearized fluxes are given by

$$\begin{aligned} F_{\alpha,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) &:= F_{\alpha,\sigma_{KL}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,\sigma_{KL}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ &+ \sum_{M \in \{K,L\}} \frac{\partial F_{\alpha,\sigma_{KL}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}). \end{aligned}$$

Fluxes reconstructions and pressure postprocessing

Fluxes reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{\sigma_{KL}} &:= F_{\alpha,\sigma_{KL}}(\mathbf{s}_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{\sigma_{KL}} &:= F_{\alpha,\sigma_{KL}}^{k-1}(\mathbf{s}_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

Phase pressures postprocessing

- Piecewise constant $\bar{p}_{\alpha,h}^{n,k,i}$ postprocessed to piecewise quadratic $p_{\alpha,h}^{n,k,i}$:

$$-\eta_{r,w}(\mathbf{s}_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{w,h}^{n,k,i}|_K) = \mathbf{d}_{w,h}^{n,k,i}|_K,$$

$$p_{w,h}^{n,k,i}(\mathbf{x}_K) = \bar{p}_{w,K}^{n,k,i},$$

$$-\eta_{r,n}(\mathbf{s}_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{n,h}^{n,k,i}|_K) = \mathbf{d}_{n,h}^{n,k,i}|_K,$$

$$p_{n,h}^{n,k,i}(\mathbf{x}_K) = \pi(\mathbf{s}_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}$$

Fluxes reconstructions and pressure postprocessing

Fluxes reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{\sigma_{KL}} &:= F_{\alpha,\sigma_{KL}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{\sigma_{KL}} &:= F_{\alpha,\sigma_{KL}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

Phase pressures postprocessing

- Piecewise constant $\bar{p}_{\alpha,h}^{n,k,i}$ postprocessed to piecewise quadratic $p_{\alpha,h}^{n,k,i}$:

$$\begin{aligned}
 -\eta_{r,w}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{w,h}^{n,k,i}|_K) &= \mathbf{d}_{w,h}^{n,k,i}|_K, \\
 p_{w,h}^{n,k,i}(\mathbf{x}_K) &= \bar{p}_{w,K}^{n,k,i},
 \end{aligned}$$

$$\begin{aligned}
 -\eta_{r,n}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{n,h}^{n,k,i}|_K) &= \mathbf{d}_{n,h}^{n,k,i}|_K, \\
 p_{n,h}^{n,k,i}(\mathbf{x}_K) &= \pi(s_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}
 \end{aligned}$$

Global pressure and Kirchhoff transform

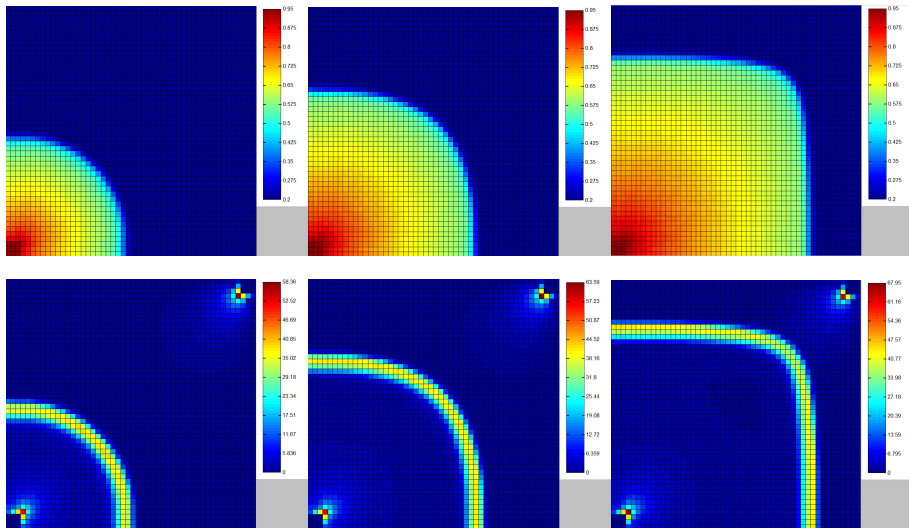
Global pressure and Kirchhoff transform postprocessing

- Piecewise quadratic global pressure and Kirchhoff transform used in the estimators:

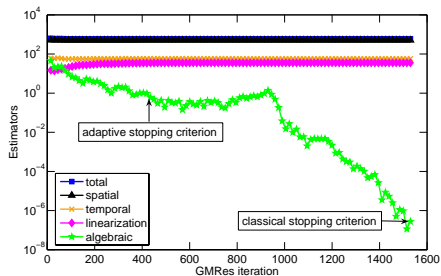
$$\begin{aligned}
 -(\eta_w(\mathbf{s}_{w,K}^{n,k,i}) + \eta_n(\mathbf{s}_{w,K}^{n,k,i})) \underline{\mathbf{K}} \nabla(\mathbf{p}_h^{n,k,i}|_K) &= (\mathbf{d}_{w,h}^{n,k,i} + \mathbf{d}_{n,h}^{n,k,i})|_K, \\
 \mathbf{p}_h^{n,k,i}(\mathbf{x}_K) &= P(\bar{\rho}_{w,K}^{n,k,i}, \mathbf{s}_{w,K}^{n,k,i}),
 \end{aligned}$$

$$\begin{aligned}
 \underline{\mathbf{K}} \nabla(\mathbf{q}_h^{n,k,i}|_K) &= \eta_n(\mathbf{s}_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(\mathbf{p}_h^{n,k,i}|_K) + \mathbf{d}_{n,h}^{n,k,i}|_K, \\
 \mathbf{q}_h^{n,k,i}(\mathbf{x}_K) &= \varphi(\mathbf{s}_{w,K}^{n,k,i})
 \end{aligned}$$

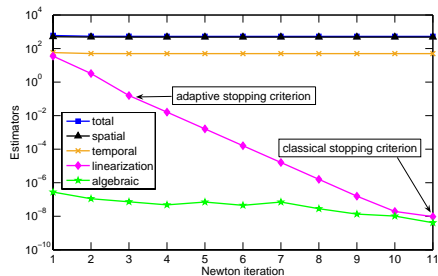
Water saturation/estimators evolution



Estimators and stopping criteria

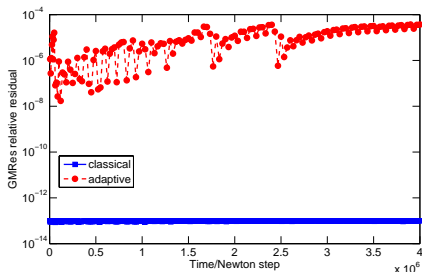


Estimators in function of GMRes iterations

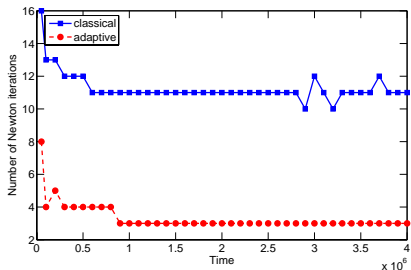


Estimators in function of Newton iterations

GMRes relative residual/Newton iterations

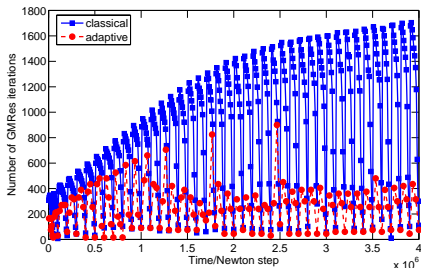


GMRes relative residual

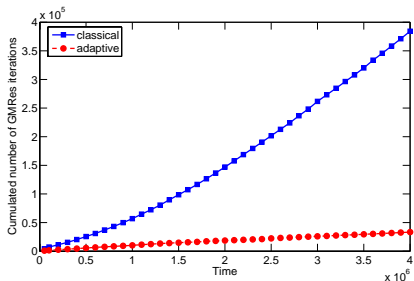


Newton iterations

GMRes iterations



Per time and Newton step



Cumulated

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Vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

Explicit saturation equation on step k

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

Vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

Explicit saturation equation on step k

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

Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} = -R_{t,D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

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

Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$\begin{aligned}
 & - \left((\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\
 & \left. + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(\mathbf{s}_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} = -R_{t,D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

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

Fluxes reconstructions

Total fluxes

$$(\mathbf{d}_{t,h}^{n,k,i} \cdot \mathbf{n}_D, 1)_\sigma := - \left((\eta_{r,w}(s_{w,h}^{n,k,i}) + \eta_{r,n}(s_{w,h}^{n,k,i})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(s_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, 1 \right)_\sigma,$$

$$((\mathbf{d}_{t,h}^{n,k,i} + \mathbf{l}_{t,h}^{n,k,i}) \cdot \mathbf{n}_D, 1)_\sigma := - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, 1 \right)_\sigma,$$

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

Wetting fluxes

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

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

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

Fluxes reconstructions

Total fluxes

$$(\mathbf{d}_{t,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_\sigma := - \left((\eta_{r,w}(s_{w,h}^{n,k,i}) + \eta_{r,n}(s_{w,h}^{n,k,i})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(s_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1} \right)_\sigma,$$

$$((\mathbf{d}_{t,h}^{n,k,i} + \mathbf{l}_{t,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1})_\sigma := - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_\sigma,$$

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

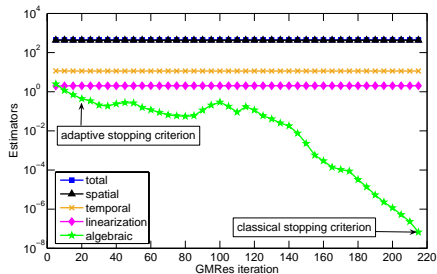
Wetting fluxes

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

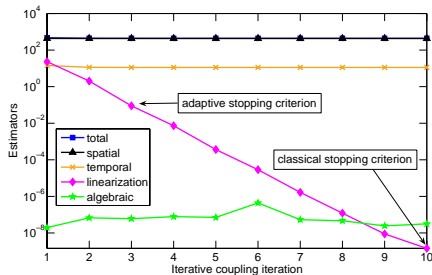
$$((\mathbf{d}_{w,h}^{n,k,i} + \mathbf{l}_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1})_\sigma := - (\eta_{r,w}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_\sigma,$$

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

Estimators and stopping criteria

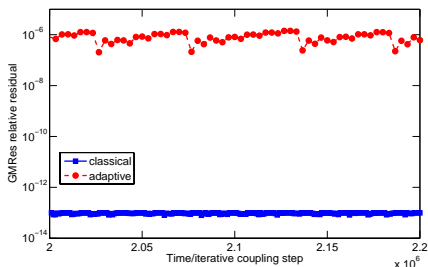


Estimators in function of GMRes iterations

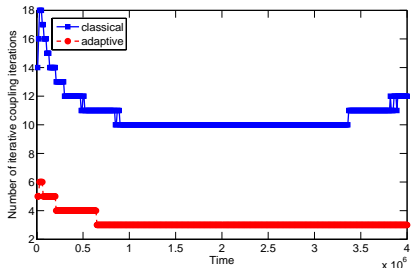


Estimators in function of iterative coupling iterations

GMRes relative residual/iterative coupling iterations

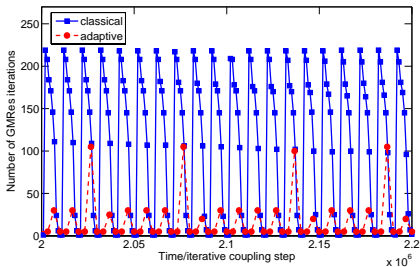


GMRes relative residual

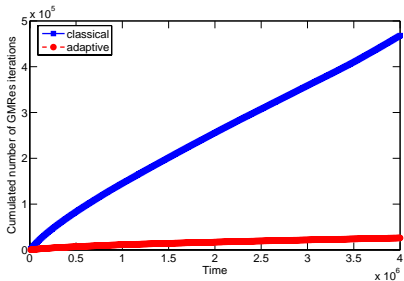


Iterative coupling iterations

GMRes iterations



Per time and iterative
coupling step



Cumulated

Outline

- 1 Introduction
- 2 Adaptive inexact Newton method
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Numerical results
- 3 Application to two-phase flow in porous media
 - A guaranteed a posteriori error estimate
 - Fully implicit cell-centered finite volumes
 - Iteratively coupled implicit pressure–explicit saturation vertex-centered finite volumes
- 4 Conclusions and future directions

Conclusions

Entire adaptivity

- only a **necessary number** of **algebraic solver iterations** on each linearization step
- only a **necessary number** of **linearization iterations**
- **“smart online decisions”**: algebraic step / linearization step / space mesh refinement / time step modification
- important **computational savings**
- guaranteed and robust error upper bound via **a posteriori estimates**

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- other coupled nonlinear systems
- convergence and optimality

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Thank you for your attention!