

Adaptive inexact Newton methods
with a posteriori stopping criteria
for nonlinear diffusion PDEs

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Outline

- 1 Introduction
- 2 Adaptive inexact Newton method
 - Quasi-linear elliptic problems
 - Approximate solution and error measure
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
- 3 Examples of application
 - Arbitrary iterative algebraic solver
 - Nonconforming FEs, fixed point/Newton, p -Laplacian
 - DGs, fixed point/Newton, quasi-linear diffusion
 - Summary
- 4 Numerical results
- 5 An extension to two-phase flows
- 6 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 and vector F^k : find U^k s.t.

$$\mathbb{A}^k U^k \approx F^k.$$

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.)

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

3 Convergence? OK $\Rightarrow U^k := U^{k,i}$. KO $\Rightarrow i := i + 1$, back to 3.2.

4 Convergence? OK \Rightarrow finish. KO $\Rightarrow k := k + 1$, back to 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 **nonlinear solver**?
- What is a good **stopping criterion** for the **linear 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)
- Moret (1989)

Stopping criteria

- engineering literature, since 1950's
- Becker, Johnson, and Rannacher (1995), multigrid st. crit.
- Arioli (2000's)

A posteriori error estimates for nonlinear problems

- Ladevèze (since 1990's), guaranteed upper bound
- Han (1994), general framework
- Verfürth (1994), residual estimates
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- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors
- Kim (2007), guaranteed estimates, loc. cons. methods

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Quasi-linear elliptic problem

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

- quasi-linear diffusion problem

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

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

Example

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

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

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

Weak formulation

Find $u \in V$ such that

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Approximate solution

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

Error measure

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

$$\mathcal{J}_{u,NC}(u_h^{k,i}) := \left\{ \sum_{K \in \mathcal{T}_h} \sum_{\theta \in \mathcal{E}_K} h_\theta^{1-q} \| \llbracket u - u_h^{k,i} \rrbracket \|_{q,\theta}^q \right\}^{1/q}$$

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

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

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

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

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
- $V(\mathcal{T}_h) := \{v \in L^p(\Omega), v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\}$

Error measure

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A posteriori error estimate

Assumption A (Total flux reconstruction)

There exists a *flux reconstruction* $\mathbf{t}_h^{k,i} \in \mathbf{H}^q(\text{div}, \Omega)$ 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. $(f_h, \mathbf{1})_K = (f, \mathbf{1})_K \quad \forall K \in \mathcal{T}_h$.

Theorem (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 $u_h^{k,i}$, $\mathbf{t}_h^{k,i}$, 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, $\|\mathbf{a}_h^{k,i}\|_q \rightarrow 0$;
- (iii) as the nonlinear solver converges, $\|\mathbf{l}_h^{k,i}\|_q \rightarrow 0$.

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

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

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Estimators

- *discretization estimator*

$$\eta_{\text{disc},K}^{k,i} := 2^{1/p} \left(\|\bar{\sigma}_h^{k,i} + \mathbf{d}_h^{k,i}\|_{q,K} + \left\{ \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|\llbracket u_h^{k,i} \rrbracket\|_{q,e}^q \right\}^{1/q} \right)$$

- *linearization estimator*

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

- *algebraic estimator*

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

- *algebraic remainder estimator*

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

- *quadrature estimator*

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

- *data oscillation estimator*

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

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

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Stopping criteria

Global stopping criteria

- stop whenever:

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

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

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

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

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

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Assumption for efficiency

Assumption C (Approximation property)

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

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

where

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

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,

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

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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Algebraic error flux reconstruction and algebraic remainder

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

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

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

- Do ν additional steps of the algebraic solver, yielding

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

- Construct the function $\rho_h^{k,i}$ from the algebraic residual vector $\mathbf{R}^{k,i+\nu}$ (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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$$\mathbb{A}^k \mathbf{U}^{k,i+\nu} = \mathbf{F}^k - \mathbf{R}^{k,i+\nu}.$$

- Construct the function $\rho_h^{k,i}$ from the algebraic residual vector $\mathbf{R}^{k,i+\nu}$ (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

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

- Independent of the algebraic solver.

Algebraic error flux reconstruction and algebraic remainder

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

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

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

- Do ν additional steps of the algebraic solver, yielding

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

- Construct the function $\rho_h^{k,i}$ from the algebraic residual vector $\mathbf{R}^{k,i+\nu}$ (lifting into appropriate discrete space).
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- Independent of the algebraic solver.

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Nonconforming finite elements for the p -Laplacian

Discretization

Find $u_h \in V_h$ such that

$$(\sigma(\nabla u_h), \nabla v_h) = (f_h, v_h) \quad \forall v_h \in V_h.$$

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

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

Nonconforming finite elements for the p -Laplacian

Discretization

Find $u_h \in V_h$ such that

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- $f_h := \Pi_0 f$
- leads to the system of **nonlinear algebraic equations**

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

Linearization

Linearization

Find $u_h^k \in V_h$ such that

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

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

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

- Newton linearization

$$\begin{aligned} \sigma^{k-1}(\xi) &:= |\nabla u_h^{k-1}|^{p-2} \xi + (p-2) |\nabla u_h^{k-1}|^{p-4} \\ &\quad (\nabla u_h^{k-1} \otimes \nabla u_h^{k-1})(\xi - \nabla u_h^{k-1}) \end{aligned}$$

- leads to the system of **linear algebraic equations**

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

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- leads to the system of **linear algebraic equations**

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

Algebraic solution

Algebraic solution

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

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

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

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

Algebraic solution

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Flux reconstructions

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

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

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

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

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

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Definition (Construction of $\bar{\sigma}_h^{k,i}$)

Set $\bar{\sigma}_h^{k,i} := \sigma(\nabla u_h^{k,i})$. 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

- $\|\mathbf{a}_h^{k,i}\|_{q,K} \rightarrow 0$ as the linear solver converges by definition.
- $\|\mathbf{l}_h^{k,i}\|_{q,K} \rightarrow 0$ 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

Lemma (Assumption C)

Assumption C holds.

Comments

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Discontinuous Galerkin for the quasi-linear diffusion

Discretization

Find $u_h \in V_h := \mathbb{P}_m(\mathcal{T}_h)$, $m \geq 1$, such that, for all $v_h \in V_h$,

$$\begin{aligned}
 & (\sigma(u_h, \nabla u_h), \nabla v_h) - \sum_{e \in \mathcal{E}_h} \{ \langle \{\sigma(u_h, \nabla u_h)\} \cdot \mathbf{n}_e, \llbracket v_h \rrbracket \rangle_e \\
 & + \theta \langle \{\underline{\mathbf{A}}(u_h) \nabla v_h\} \cdot \mathbf{n}_e, \llbracket u_h \rrbracket \rangle_e \} + \sum_{e \in \mathcal{E}_h} \langle \bar{\alpha}_e h_e^{-1} \llbracket u_h \rrbracket, \llbracket v_h \rrbracket \rangle_e = (f, v_h).
 \end{aligned}$$

- $\theta \in \{-1, 0, 1\}$
- $\bar{\alpha}_e := \|\underline{\mathbf{A}}\|_{L^\infty(\mathbb{R})} \chi_e$, χ_e large enough
- leads to the system of nonlinear algebraic equations

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

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- leads to the system of **nonlinear algebraic equations**

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

Linearization

Linearization

Find $u_h^k \in V_h$ such that, for all $K \in \mathcal{T}_h$ and all $j \in \mathcal{C}_K := \{1, \dots, \dim(\mathbb{P}_m(K))\}$,

$$(\sigma^{k-1}(u_h^k, \nabla u_h^k), \nabla \psi_{K,j}) - \sum_{e \in \mathcal{E}_h} \{ \langle \{\sigma^{k-1}(u_h^k, \nabla u_h^k)\} \cdot \mathbf{n}_e, [\psi_{K,j}] \rangle_e \\ + \theta \langle \{\underline{\mathbf{A}}^{k-1}(u_h^k) \nabla \psi_{K,j}\} \cdot \mathbf{n}_e, [u_h^k] \rangle_e \} + \sum_{e \in \mathcal{E}_h} \langle \bar{\alpha}_e h_e^{-1} [u_h^k], [\psi_{K,j}] \rangle_e = (f, \psi_{K,j}).$$

- $u_h^0 \in V_h$ yields the initial vector U^0
- fixed-point linearization $\sigma^{k-1}(v, \xi) := \underline{\mathbf{A}}(u_h^{k-1})\xi$
- Newton linearization

$$\sigma^{k-1}(v, \xi) := \underline{\mathbf{A}}(u_h^{k-1})\xi + (v - u_h^{k-1})\partial_v \underline{\mathbf{A}}(u_h^{k-1})\nabla u_h^{k-1},$$

$$\underline{\mathbf{A}}^{k-1}(v) := \underline{\mathbf{A}}(u_h^{k-1}) + \partial_v \underline{\mathbf{A}}(u_h^{k-1})(v - u_h^{k-1})$$

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Linearization

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Algebraic solution

Algebraic solution

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

$$\begin{aligned}
 & (\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i}), \nabla \psi_{K,j}) - \sum_{e \in \mathcal{E}_h} \{ \langle \{\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i})\} \cdot \mathbf{n}_e, [\psi_{K,j}] \rangle_e \\
 & + \theta \langle \{\underline{\mathbf{A}}^{k-1}(u_h^{k,i}) \nabla \psi_{K,j}\} \cdot \mathbf{n}_e, [u_h^{k,i}] \rangle_e \} + \sum_{e \in \mathcal{E}_h} \langle \bar{\alpha}_e h_e^{-1} [u_h^{k,i}], [\psi_{K,j}] \rangle_e \\
 & = (f, \psi_{K,j}) - R_{K,j}^{k,i}.
 \end{aligned}$$

- algebraic residual vector $R^{k,i} = \{R_{K,j}^{k,i}\}_{K \in \mathcal{T}_h, j \in \mathcal{C}_K}$
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Flux reconstructions

Definition (Construction of $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \in \mathbf{RTN}_l(\mathcal{T}_h)$, $l := m-1/m$)

For all $K \in \mathcal{T}_h$ and all $e \in \mathcal{E}_K$,

$$\langle (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \cdot \mathbf{n}_e, q_h \rangle_e := \langle -\{\{\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i})\}\} \cdot \mathbf{n}_e + \bar{\alpha}_e h_e^{-1} \llbracket u_h^{k,i} \rrbracket, q_h \rangle_e,$$

$$(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}, \mathbf{r}_h)_K := -(\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i}), \mathbf{r}_h)_K$$

$$+ \theta \sum_{e \in \mathcal{E}_K} w_e \langle \underline{\mathbf{A}}^{k-1}(u_h^{k,i}) \mathbf{r}_h \cdot \mathbf{n}_e, \llbracket u_h^{k,i} \rrbracket \rangle_e,$$

for all $q_h \in \mathbb{P}_l(e)$ and all $\mathbf{r}_h \in [\mathbb{P}_{l-1}(K)]^d$.

Definition (Construction of $\mathbf{d}_h^{k,i} \in \mathbf{RTN}_l(\mathcal{T}_h)$, $l := m-1$ or $l := m$)

For all $K \in \mathcal{T}_h$ and all $e \in \mathcal{E}_K$,

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Verification of the assumptions – upper bound

Definition (Construction of $f_h, \bar{\sigma}_h^{k,i}$)

Set $f_h := \Pi_I f$ and $\bar{\sigma}_h^{k,i} := \mathbf{I}_I^{\text{RTN}}(\sigma(u_h^{k,i}, \nabla u_h^{k,i}))$.

Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

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

Verification of the assumptions – upper bound

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Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

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

Verification of the assumptions – upper bound

Definition (Construction of $f_h, \bar{\sigma}_h^{k,i}$)

Set $f_h := \Pi_I f$ and $\bar{\sigma}_h^{k,i} := \mathbf{I}_I^{\text{RTN}}(\sigma(u_h^{k,i}, \nabla u_h^{k,i}))$.

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Assumptions A and B hold.

Comments

- $\|\mathbf{a}_h^{k,i}\|_{q,K} \rightarrow 0$ as the linear solver converges by definition.
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Verification of the assumptions – efficiency

Lemma (Assumption C)

Assumption C holds.

Comments

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

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 - DGs, fixed point/Newton, quasi-linear diffusion
 - **Summary**
- 4 Numerical results
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- 6 Conclusions and future directions

Summary

Discretization methods

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

Linearizations

- fixed point
- Newton

Linear solvers

- independent of the linear solver

... all Assumptions A to C verified

Summary

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Numerical experiment I

Model problem

- p -Laplacian

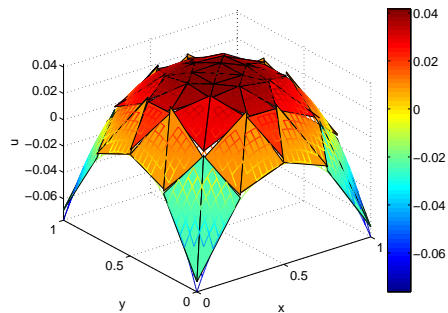
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

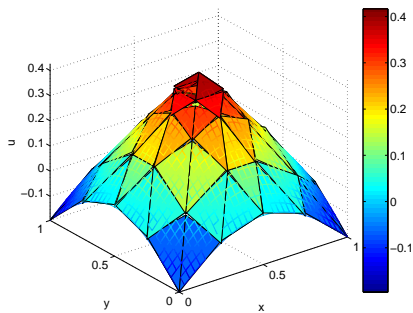
$$u(x, y) = -\frac{p-1}{p} \left((x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left(\frac{1}{2} \right)^{\frac{p}{p-1}}$$

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

Analytical and approximate solutions

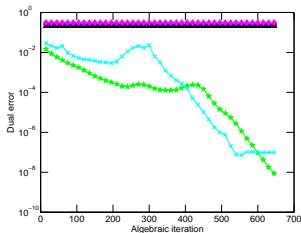


Case $p = 1.5$

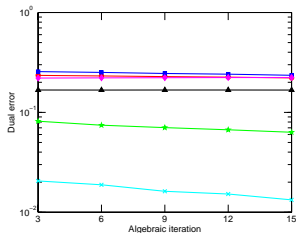


Case $p = 10$

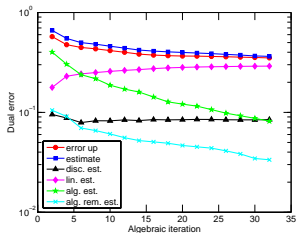
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

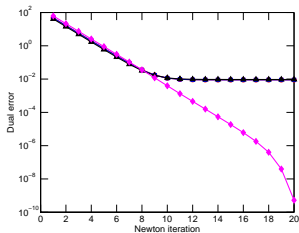


inexact Newton

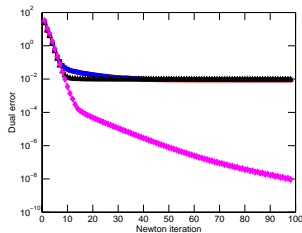


ad. inexact Newton

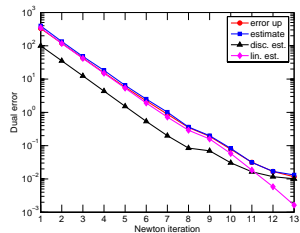
Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh



Newton

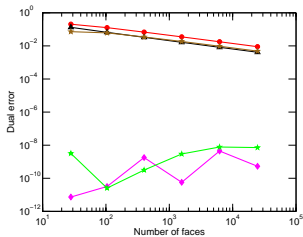


inexact Newton

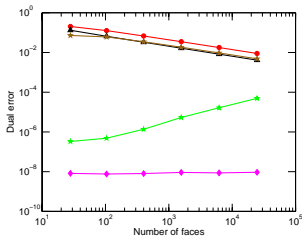


ad. inexact Newton

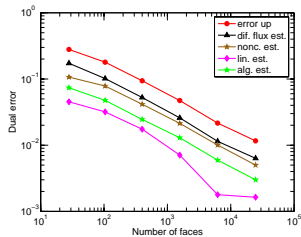
Error and estimators, $p = 10$



Newton

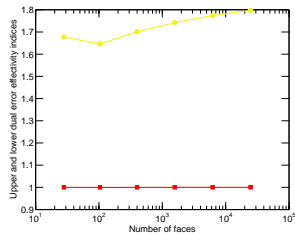


inexact Newton

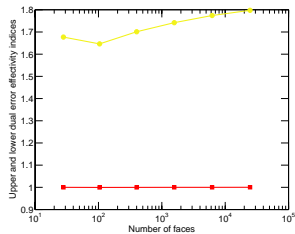


ad. inexact Newton

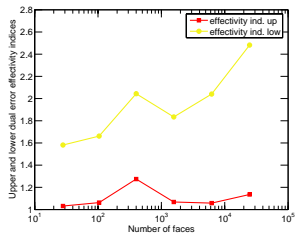
Effectivity indices, $p = 10$



Newton

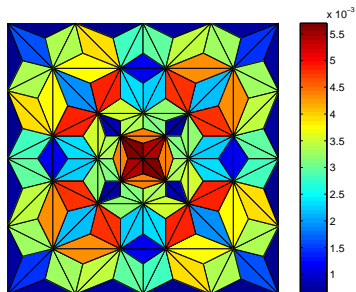


inexact Newton

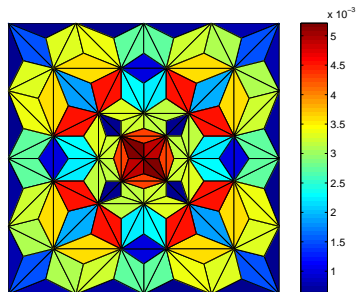


ad. inexact Newton

Error distribution, $p = 10$

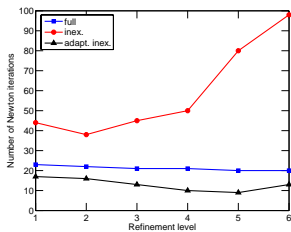


Estimated error distribution

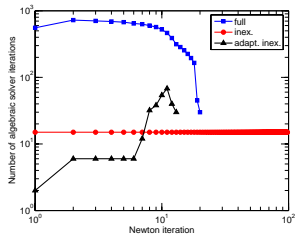


Exact error distribution

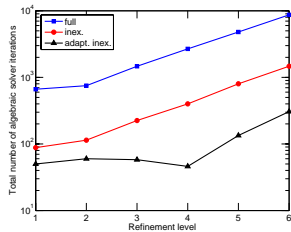
Newton and algebraic iterations, $p = 10$



Newton it. / refinement

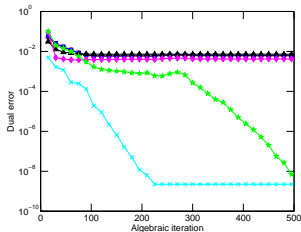


alg. it. / Newton step

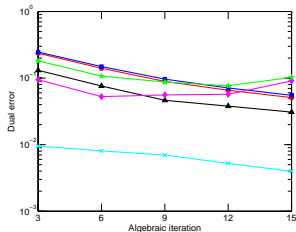


alg. it. / refinement

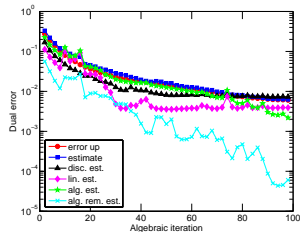
Error and estimators as a function of CG iterations, $\rho = 1.5$, 6th level mesh, 1st Newton step.



Newton

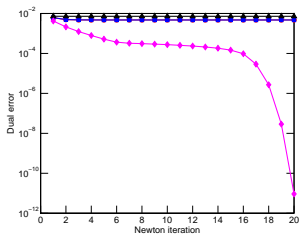


inexact Newton

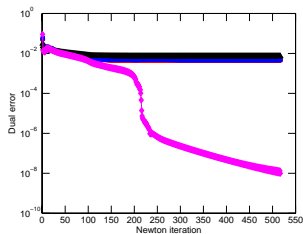


ad. inexact Newton

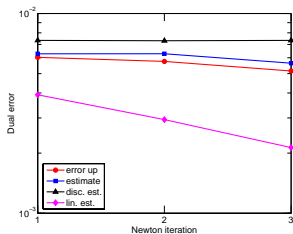
Error and estimators as a function of Newton iterations, $p = 1.5$, 6th level mesh



Newton

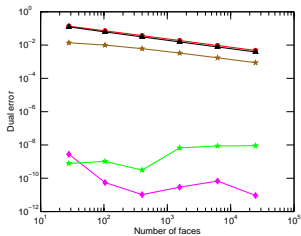


inexact Newton

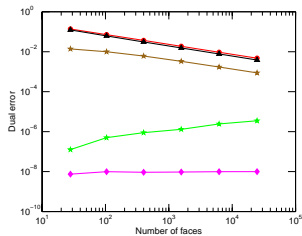


ad. inexact Newton

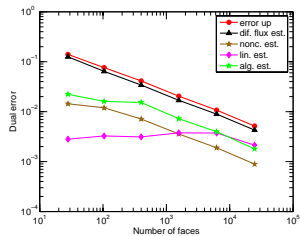
Error and estimators, $p = 1.5$



Newton

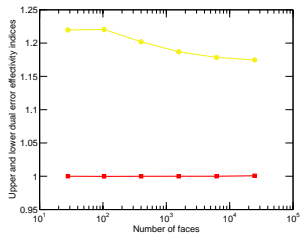


inexact Newton

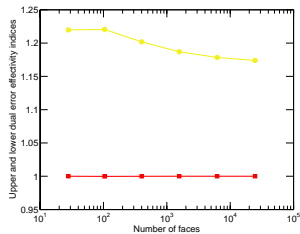


ad. inexact Newton

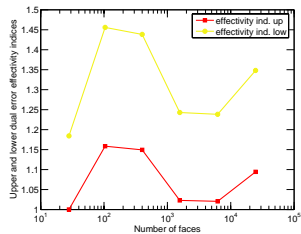
Effectivity indices, $p = 1.5$



Newton

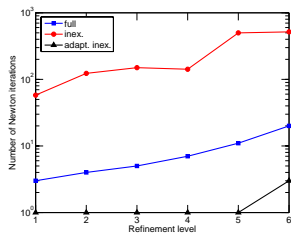


inexact Newton

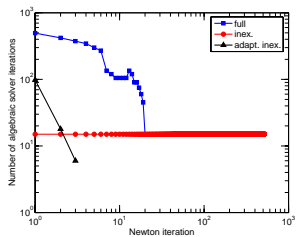


ad. inexact Newton

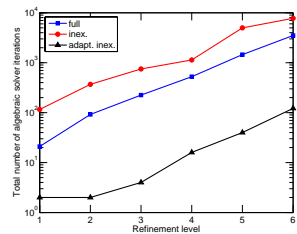
Newton and algebraic iterations, $p = 1.5$



Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p -Laplacian

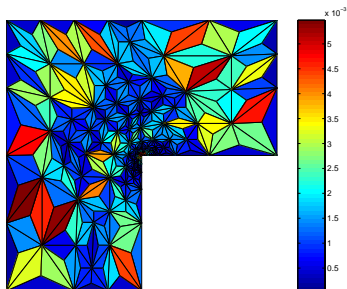
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

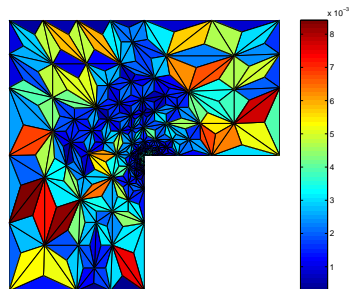
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

Error distribution on an adaptively refined mesh

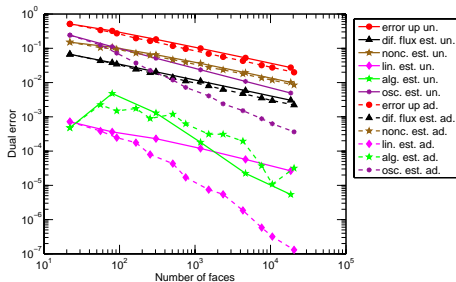


Estimated error distribution

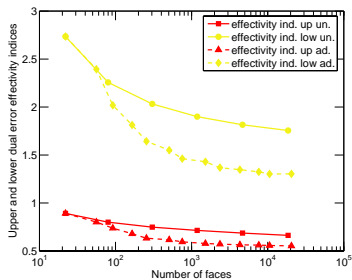


Exact error distribution

Estimated and actual errors and the effectivity index



Estimated and actual errors



Effectivity index

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Two-phase flow in porous media

Two-phase flow in porous media

$$\begin{aligned} \partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \mathbf{u}_\alpha &= \mathbf{q}_\alpha, & \alpha \in \{\mathbf{n}, \mathbf{w}\}, \\ -\frac{k_{r,\alpha}(\mathbf{s}_w)}{\mu_\alpha} \mathbf{K}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{\mathbf{n}, \mathbf{w}\}, \\ \mathbf{s}_n + \mathbf{s}_w &= \mathbf{1}, \\ \rho_n - \rho_w &= \rho_c(\mathbf{s}_w) \end{aligned}$$

Mathematical issues

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

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- coupled system
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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 $(s_{\alpha,h\tau}^{k,i}, p_{\alpha,h\tau}^{k,i})$. Then

$$\| (s_{\alpha} - s_{\alpha,h\tau}^{k,i}, p_{\alpha} - p_{\alpha,h\tau}^{k,i}) \|_{l_n} \leq \eta_{\text{sp},\alpha}^{n,k,i} + \eta_{\text{tm},\alpha}^{n,k,i} + \eta_{\text{lin},\alpha}^{n,k,i} + \eta_{\text{alg},\alpha}^{n,k,i}$$

Error components

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

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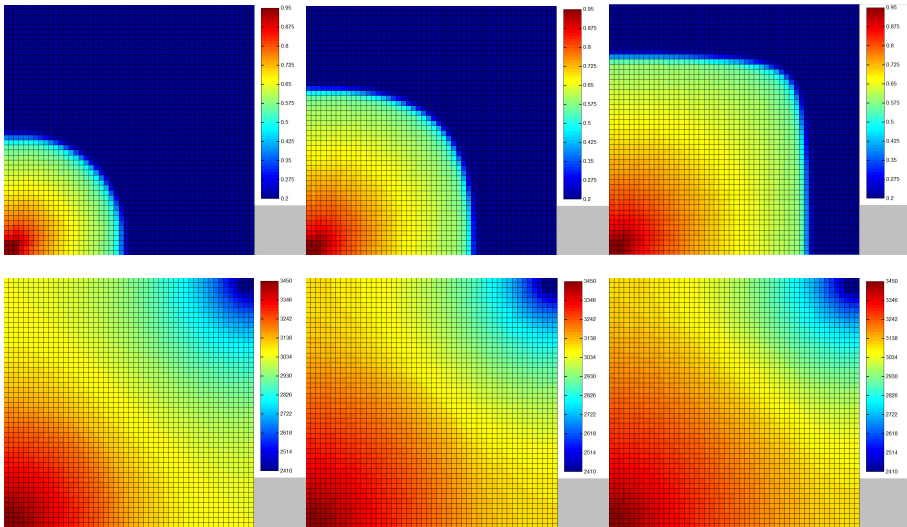
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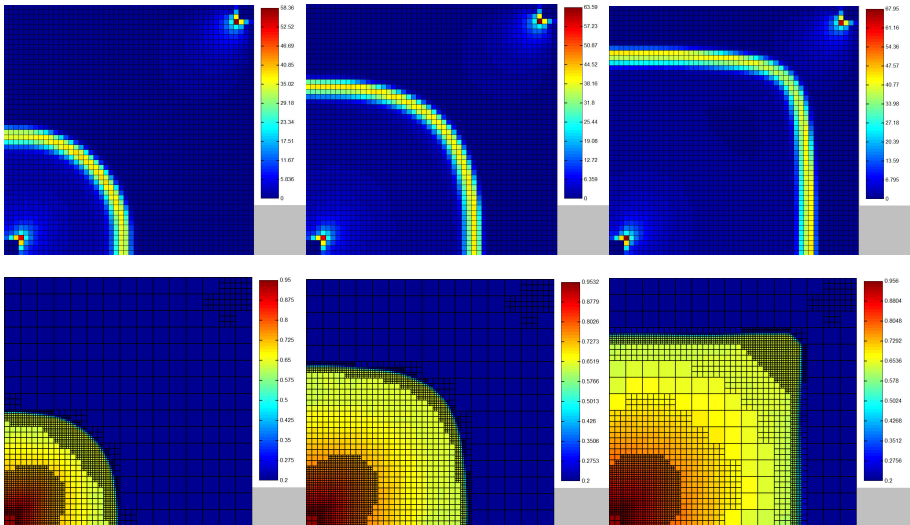
Error components

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

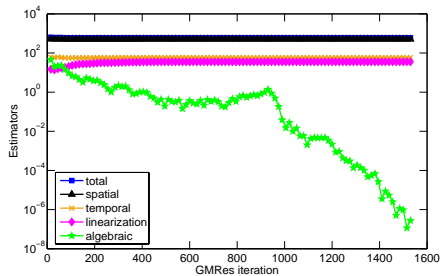
Water saturation/water pressure evolution



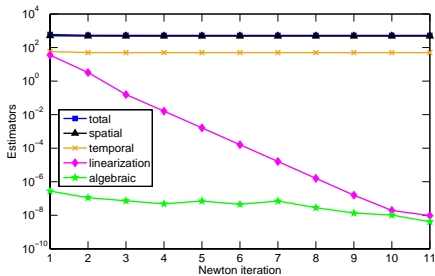
Estimators/meshes evolution



Estimators and stopping criteria

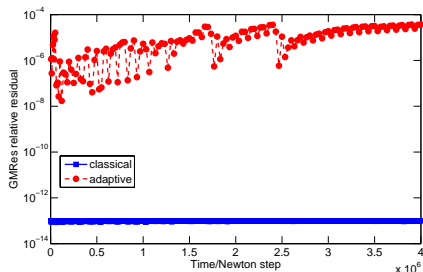


Estimators in function of
GMRes iterations

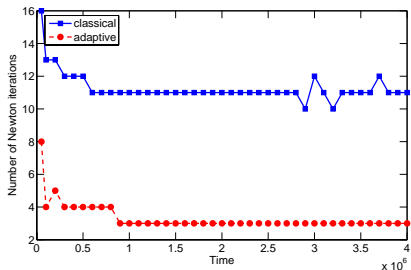


Estimators in function of
Newton iterations

GMRes relative residual/Newton iterations

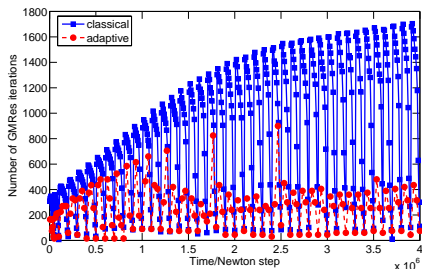


GMRes relative residual

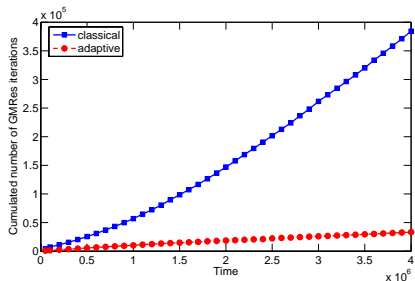


Newton iterations

GMRes iterations



Per time and Newton step



Cumulated

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Adaptive inexact Newton method

- 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
- important **computational savings**
- guaranteed and robust upper bound via **a posteriori error estimates**

Future directions

- other coupled nonlinear systems
- convergence and optimality

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Bibliography

- ERN A., VOHRALÍK M., Adaptive inexact Newton methods for discretizations of nonlinear diffusion PDEs. I. General theory and a posteriori stopping criteria, HAL Preprint 00681422 & Adaptive inexact Newton methods for discretizations of nonlinear diffusion PDEs. II. Applications, HAL Preprint 00681426.
- JIRÁNEK P., STRAKOŠ Z., VOHRALÍK M., A posteriori error estimates including algebraic error and stopping criteria for iterative solvers. *SIAM J. Sci. Comput.* **32** (2010), 1567–1590.
- EL ALAOU L., ERN A., VOHRALÍK M., Guaranteed and robust a posteriori error estimates and balancing discretization and linearization errors for monotone nonlinear problems. *Comput. Methods Appl. Mech. Engrg.* **200** (2011), 2782–2795.

Thank you for your attention!