

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

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Inexact iterative linearization

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 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.

$$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$
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 - 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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- 2 Laplace equation
 - A guaranteed a posteriori error estimate
 - Polynomial-degree-robust local efficiency
 - Application and numerical results
- 3 Quasi-linear elliptic problems
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- 4 Two-phase flow in porous media
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- 5 Conclusions and future directions

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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
- Hackbusch and Reusken (1989), damping and multigrid
- Deuffhard (1990's, 2004 book), adaptivity

Stopping criteria for algebraic solvers

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

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

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A posteriori error estimate, $-\Delta u = f$ in Ω , $u = 0$ on $\partial\Omega$

Theorem (A guaranteed a posteriori error estimate)

- Let $u \in H_0^1(\Omega)$ be the weak solution,
- $u_h \in H^1(\mathcal{T}_h) := \{v \in L^2(\Omega), v|_K \in H^1(K) \forall K \in \mathcal{T}_h\}$ be *arbitrary*,
- $s_h \in H_0^1(\Omega)$ and $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$ with $(\nabla \cdot \sigma_h, 1)_K = (f, 1)_K$ for all $K \in \mathcal{T}_h$ be *arbitrary*.

Then
$$\|\nabla(u - u_h)\|^2 \leq \sum_{K \in \mathcal{T}_h} \left(\|\nabla u_h + \sigma_h\|_K + \frac{h_K}{\pi} \|f - \nabla \cdot \sigma_h\|_K \right)^2 + \sum_{K \in \mathcal{T}_h} \|\nabla(u_h - s_h)\|_K^2.$$

Proof (Spirit of Prager–Synge (1947)).

- define $s \in H_0^1(\Omega)$ by

$$(\nabla s, \nabla v) = (\nabla u_h, \nabla v) \quad \forall v \in H_0^1(\Omega)$$

- develop (Pythagoras)

$$\|\nabla(u - u_h)\|^2 = \|\nabla(u - s)\|^2 + \|\nabla(s - u_h)\|^2$$

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Proof (continuation).

- projection:

$$\|\nabla(u - u_h)\|^2 = \underbrace{\sup_{\varphi \in H_0^1(\Omega); \|\nabla\varphi\|=1} (\nabla(u - u_h), \nabla\varphi)^2}_{\text{dual norm of the residual}} + \underbrace{\min_{v \in H_0^1(\Omega)} \|\nabla(v - u_h)\|^2}_{\text{distance of } u_h \text{ to } H_0^1(\Omega)}$$

- minimization upper bound:

$$\min_{v \in H_0^1(\Omega)} \|\nabla(v - u_h)\| \leq \|\nabla(u_h - s_h)\|$$

- weak solution definition, equilibrated flux:

$$(\nabla(u - u_h), \nabla\varphi) = (f, \varphi) - (\nabla u_h, \nabla\varphi) = (f - \nabla \cdot \sigma_h, \varphi) - (\nabla u_h + \sigma_h, \nabla\varphi)$$

- Cauchy–Schwarz and Poincaré inequalities:

$$-(\nabla u_h + \sigma_h, \nabla\varphi) \leq \sum_{K \in \mathcal{T}_h} \|\nabla u_h + \sigma_h\|_K \|\nabla\varphi\|_K,$$

$$(f - \nabla \cdot \sigma_h, \varphi) = \sum_{K \in \mathcal{T}_h} (f - \nabla \cdot \sigma_h, \varphi - \varphi_K)_K \leq \sum_{K \in \mathcal{T}_h} \frac{h_K}{\pi} \|f - \nabla \cdot \sigma_h\|_K \|\nabla\varphi\|_K$$

Potential and flux reconstruction

Ideally

$$\sigma_h := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h, \nabla \cdot \mathbf{v}_h = \Pi_{Q_h} f} \|\nabla u_h + \mathbf{v}_h\|$$

$$s_h := \arg \min_{v_h \in V_h} \|\nabla(u_h - v_h)\|$$

- too expensive

Partition of unity

$$\sigma_h^a := \arg \min_{\mathbf{v}_h \in \mathbf{V}_h^a, \nabla \cdot \mathbf{v}_h = ?} \|\psi_a \nabla u_h + \mathbf{v}_h\|_{\omega_a}$$

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- $\sigma_h := \sum_{\mathbf{a} \in \mathcal{V}_h} \sigma_h^{\mathbf{a}}, \quad s_h := \sum_{\mathbf{a} \in \mathcal{V}_h} s_h^{\mathbf{a}}$

- local minimizations

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Practical flux reconstruction

Assumption A (Galerkin orthogonality)

There holds

$$(\nabla u_h, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = (f, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} \quad \forall \mathbf{a} \in \mathcal{V}_h^{\text{int}}.$$

Definition (Construction of σ_h , Destuynder and Métivet (1999) & Braess and Schöberl (2008))

Let **Assumption A** be satisfied. For each $\mathbf{a} \in \mathcal{V}_h$, prescribe $\varsigma_h^{\mathbf{a}} \in \mathbf{V}_h^{\mathbf{a}}$ and $\bar{r}_h^{\mathbf{a}} \in Q_h^{\mathbf{a}}$ by solving the local MFE problem

$$\begin{aligned} (\varsigma_h^{\mathbf{a}}, \mathbf{v}_h)_{\omega_{\mathbf{a}}} - (\bar{r}_h^{\mathbf{a}}, \nabla \cdot \mathbf{v}_h)_{\omega_{\mathbf{a}}} &= -(\psi_{\mathbf{a}} \nabla u_h, \mathbf{v}_h)_{\omega_{\mathbf{a}}} & \forall \mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}}, \\ (\nabla \cdot \varsigma_h^{\mathbf{a}}, q_h)_{\omega_{\mathbf{a}}} &= (\psi_{\mathbf{a}} f - \nabla \psi_{\mathbf{a}} \cdot \nabla u_h, q_h)_{\omega_{\mathbf{a}}} & \forall q_h \in Q_h^{\mathbf{a}}, \end{aligned}$$

with $\mathbf{V}_h^{\mathbf{a}} \times Q_h^{\mathbf{a}}$ mixed finite element spaces (hom. Neumann BC for $\mathbf{a} \in \mathcal{V}_h^{\text{int}}$, hom. Dirichlet BC on $\partial\omega_{\mathbf{a}} \cap \partial\Omega$ for $\mathbf{a} \in \mathcal{V}_h^{\text{ext}}$). Set

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with $\mathbf{V}_h^{\mathbf{a}} \times Q_h^{\mathbf{a}}$ mixed finite element spaces (hom. Neumann BC for $\mathbf{a} \in \mathcal{V}_h^{\text{int}}$, hom. Dirichlet BC on $\partial\omega_{\mathbf{a}} \cap \partial\Omega$ for $\mathbf{a} \in \mathcal{V}_h^{\text{ext}}$). Set

$$\sigma_h := \sum_{\mathbf{a} \in \mathcal{V}_h} \varsigma_h^{\mathbf{a}}.$$

Practical potential reconstruction ($d = 2$)

Definition (Construction of s_h)

For each $\mathbf{a} \in \mathcal{V}_h$, prescribe $\mathbf{s}_h^{\mathbf{a}} \in \mathbf{V}_h^{\mathbf{a}}$ and $\bar{\mathbf{r}}_h^{\mathbf{a}} \in Q_h^{\mathbf{a}}$ by solving the local MFE problem

$$\begin{aligned} (\mathbf{s}_h^{\mathbf{a}}, \mathbf{v}_h)_{\omega_{\mathbf{a}}} - (\bar{\mathbf{r}}_h^{\mathbf{a}}, \nabla \cdot \mathbf{v}_h)_{\omega_{\mathbf{a}}} &= -(\mathbf{R}_{\frac{\pi}{2}} \nabla(\psi_{\mathbf{a}} U_h), \mathbf{v}_h)_{\omega_{\mathbf{a}}} \quad \forall \mathbf{v}_h \in \mathbf{V}_h^{\mathbf{a}}, \\ (\nabla \cdot \mathbf{s}_h^{\mathbf{a}}, q_h)_{\omega_{\mathbf{a}}} &= (\mathbf{0}, q_h)_{\omega_{\mathbf{a}}} \quad \forall q_h \in Q_h^{\mathbf{a}}, \end{aligned}$$

with $\mathbf{V}_h^{\mathbf{a}} \times Q_h^{\mathbf{a}}$ mixed finite element spaces (hom. Neumann BC for all $\mathbf{a} \in \mathcal{V}_h$). Set

$$\begin{aligned} -\mathbf{R}_{\frac{\pi}{2}} \nabla s_h^{\mathbf{a}} &= \mathbf{s}_h^{\mathbf{a}}, \\ s_h^{\mathbf{a}} &= 0 \text{ on } \partial\omega_{\mathbf{a}}, \\ s_h &:= \sum_{\mathbf{a} \in \mathcal{V}_h} s_h^{\mathbf{a}}. \end{aligned}$$

Remark

- The same problems, only RHS/BC different.

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Outline

- 1 Bibliography
- 2 Laplace equation
 - A guaranteed a posteriori error estimate
 - **Polynomial-degree-robust local efficiency**
 - Application and numerical results
- 3 Quasi-linear elliptic problems
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Flux reconstruction

Theorem (Continuous efficiency, Carstensen & Funken (1999), Braess, Pillwein, and Schöberl (2009))

Let u be the weak solution and let $u_h \in H^1(\mathcal{T}_h)$ be *arbitrary*. Let $\mathbf{a} \in \mathcal{V}_h$ and let $r_{\mathbf{a}} \in H_*^1(\omega_{\mathbf{a}})$ solve

$$(\nabla r_{\mathbf{a}}, \nabla v)_{\omega_{\mathbf{a}}} = -(\psi_{\mathbf{a}} \nabla u_h, \nabla v)_{\omega_{\mathbf{a}}} + (\psi_{\mathbf{a}} f - \nabla \psi_{\mathbf{a}} \cdot \nabla u_h, v)_{\omega_{\mathbf{a}}} \quad \forall v \in H_*^1(\omega_{\mathbf{a}})$$

with $H_*^1(\omega_{\mathbf{a}}) := \{v \in H^1(\omega_{\mathbf{a}}); (v, 1)_{\omega_{\mathbf{a}}} = 0 / v = 0 \text{ on } \partial\omega_{\mathbf{a}} \cap \partial\Omega\}$.
Then there exists a constant $C_{\text{cont,PF}} > 0$ *only depending on the shape-regularity parameter $\kappa_{\mathcal{T}}$* such that

$$\|\nabla r_{\mathbf{a}}\|_{\omega_{\mathbf{a}}} \leq C_{\text{cont,PF}} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}}.$$

Potential reconstruction ($d = 2$)

Assumption B (Weak continuity)

There holds $\langle \llbracket u_h \rrbracket, 1 \rangle_e = 0 \quad \forall e \in \mathcal{E}_h.$

Theorem (Continuous efficiency)

Let u be the weak solution and let $u_h \in H^1(\mathcal{T}_h)$ satisfying Assumption B be arbitrary. Let $\mathbf{a} \in \mathcal{V}_h$ and let $r_{\mathbf{a}} \in H_*^1(\omega_{\mathbf{a}})$ solve

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with $H_*^1(\omega_{\mathbf{a}}) := \{v \in H^1(\omega_{\mathbf{a}}); (v, 1)_{\omega_{\mathbf{a}}} = 0\}$. Then there exists a constant $C_{\text{cont,bPF}} > 0$ only depending on the shape-regularity parameter $\kappa_{\mathcal{T}}$ such that

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Mixed finite elements stability ($d = 2$)

Theorem (MFE stability, Braess, Pillwein, and Schöberl (2009))

Let u be the weak solution and let u_h and f be *piecewise polynomial*. Consider *corresponding* polynomial degree MFE reconstructions. Then there exists a constant $C_{\text{st}} > 0$ *only depending* on the shape-regularity parameter $\kappa_{\mathcal{T}}$ such that

$$\|\varsigma_h^{\mathbf{a}} + \tau_h^{\mathbf{a}}\|_{\omega_{\mathbf{a}}} \leq C_{\text{st}} \|\nabla r_{\mathbf{a}}\|_{\omega_{\mathbf{a}}},$$

with $\tau_h^{\mathbf{a}} = \psi_{\mathbf{a}} \nabla u_h$ for the flux reconstruction and $\varsigma_h^{\mathbf{a}} = \mathbf{R}_{\frac{\pi}{2}} \nabla(\psi_{\mathbf{a}} u_h)$ for the potential reconstruction.

Polynomial-degree-robust efficiency

Theorem (Polynomial-degree-robust efficiency)

Let u be the weak solution and let u_h and f be piecewise polynomial. Let u_h satisfy [Assumptions A](#) and [B](#). Then, for corresponding polynomial degree MFE reconstructions,

$$\|\nabla u_h + \sigma_h\|_K \leq C_{\text{st}} C_{\text{cont,PF}} \sum_{\mathbf{a} \in \mathcal{V}_K} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}},$$

$$\|\nabla(u_h - s_h)\|_K \leq C_{\text{st}} C_{\text{cont,bPF}} \sum_{\mathbf{a} \in \mathcal{V}_K} \|\nabla(u - u_h)\|_{\omega_{\mathbf{a}}}.$$

Remarks

- C_{st} can be **bounded** by solving the local Neumann problems by a **conforming FEs**
- **maximal overestimation factor guaranteed**

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Outline

- 1 Bibliography
- 2 Laplace equation
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 - **Application and numerical results**
- 3 Quasi-linear elliptic problems
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 - Stopping criteria and efficiency
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Conforming finite elements

Conforming finite elements

Find $u_h \in V_h$ such that

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

- $V_h := \mathbb{P}_p(\mathcal{T}_h) \cap H_0^1(\Omega)$, $p \geq 1$
- **Assumption A**: take $v_h = \psi_a$
- $V_h \subset H_0^1(\Omega)$: $s_h := u_h$, no need for **Assumption B**

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- Assumption B: building requirement for the space V_h

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Discontinuous Galerkin finite elements

Discontinuous Galerkin finite elements

Find $u_h \in V_h$ such that

$$\sum_{K \in \mathcal{T}_h} (\nabla u_h, \nabla v_h)_K - \sum_{e \in \mathcal{E}_h} \{ \langle \{\nabla u_h\} \cdot \mathbf{n}_e, [v_h] \rangle_e + \theta \langle \{\nabla v_h\} \cdot \mathbf{n}_e, [u_h] \rangle_e \} \\ + \sum_{e \in \mathcal{E}_h} \langle \alpha h_e^{-1} [u_h], [v_h] \rangle_e = (f, v_h) \quad \forall v_h \in V_h$$

- $V_h := \mathbb{P}_p(\mathcal{T}_h)$, $p \geq 1$
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Mixed finite elements

Mixed finite elements

Find a couple $(\sigma_h, \bar{u}_h) \in \mathbf{V}_h \times Q_h$ such that

$$\begin{aligned} (\sigma_h, \mathbf{v}_h) - (\bar{u}_h, \nabla \cdot \mathbf{v}_h) &= 0 & \forall \mathbf{v}_h \in \mathbf{V}_h, \\ (\nabla \cdot \sigma_h, q_h) &= (f, q_h) & \forall q_h \in Q_h. \end{aligned}$$

- postprocessed solution $u_h \in V_h$, $V_h := \mathbb{P}_\rho(\mathcal{T}_h)$, $\rho \geq 1$, $v_h \in V_h$ satisfy

$$\langle \llbracket v_h \rrbracket, q_h \rangle_e = 0 \quad \forall q_h \in \mathbb{P}_{\rho'}(e), \forall e \in \mathcal{E}_h$$

- Assumption A:** no need for flux reconstruction, σ_h comes from the discretization
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Numerics: discontinuous Galerkin

Model problem

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega :=]0, 1[\times]0, 1[, \\ u &= u_D & \text{on } \partial\Omega \end{aligned}$$

Exact solution

$$\begin{aligned} u(\mathbf{x}) &= (c_1 + c_2(1 - x_1) + e^{-\alpha x_1})(c_1 + c_2(1 - x_2) + e^{-\alpha x_2}) \\ c_1 &= -e^{-\alpha}, \quad c_2 = -1 - c_1, \quad \alpha = 10 \end{aligned}$$

Discretization

incomplete interior penalty discontinuous Galerkin method

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Estimates, errors, effectivity indices (calc. V. Dolejší)

h	p	$\ u - u_h\ $	$\ \nabla(u - u_h)\ $	$\ \nabla u_h + \sigma_h\ $	$\frac{h_K}{\pi} \ f - \nabla \cdot \sigma_h\ $	$\ \nabla(u_h - s_h)\ $	η	l_{eff}
1.3E-01	1	1.39E-02	4.98E-01	5.32E-01	4.34E-02	3.52E-02	5.71E-01	1.15
6.3E-02		3.85E-03	2.67E-01	2.80E-01	6.29E-03	1.96E-02	2.86E-01	1.07
(EOC)		(1.85)	(0.90)	(0.93)	(2.79)	(0.85)	(1.00)	
3.1E-02		9.90E-04	1.37E-01	1.42E-01	8.19E-04	1.01E-02	1.43E-01	1.04
(EOC)		(1.96)	(0.97)	(0.98)	(2.94)	(0.96)	(1.00)	
1.6E-02		2.49E-04	6.89E-02	7.12E-02	1.03E-04	5.01E-03	7.15E-02	1.04
(EOC)		(1.99)	(0.99)	(0.99)	(2.99)	(1.01)	(1.00)	
1.3E-01	2	2.08E-03	9.38E-02	9.48E-02	8.83E-03	1.27E-02	1.03E-01	1.10
6.3E-02		4.02E-04	2.61E-02	2.62E-02	6.37E-04	4.07E-03	2.71E-02	1.04
(EOC)		(2.37)	(1.84)	(1.85)	(3.79)	(1.65)	(1.93)	
3.1E-02		8.26E-05	6.75E-03	6.76E-03	4.13E-05	1.19E-03	6.90E-03	1.02
(EOC)		(2.28)	(1.95)	(1.96)	(3.95)	(1.77)	(1.97)	
1.6E-02		1.85E-05	1.71E-03	1.71E-03	2.61E-06	3.22E-04	1.74E-03	1.02
(EOC)		(2.16)	(1.98)	(1.99)	(3.99)	(1.88)	(1.99)	
1.3E-01	3	2.29E-04	1.55E-02	1.51E-02	1.38E-03	2.36E-03	1.66E-02	1.07
6.3E-02		1.65E-05	2.20E-03	2.15E-03	4.98E-05	3.85E-04	2.23E-03	1.01
(EOC)		(3.80)	(2.81)	(2.81)	(4.79)	(2.62)	(2.89)	
3.1E-02		1.08E-06	2.85E-04	2.80E-04	1.62E-06	5.25E-05	2.86E-04	1.01
(EOC)		(3.94)	(2.95)	(2.94)	(4.94)	(2.87)	(2.97)	
1.6E-02		6.77E-08	3.58E-05	3.54E-05	5.10E-08	6.62E-06	3.60E-05	1.01
(EOC)		(3.99)	(2.99)	(2.98)	(4.99)	(2.99)	(2.99)	
1.3E-01	4	2.64E-05	2.28E-03	2.17E-03	1.69E-04	3.46E-04	2.37E-03	1.04
6.3E-02		1.08E-06	1.63E-04	1.57E-04	3.05E-06	3.25E-05	1.63E-04	1.00
(EOC)		(4.61)	(3.80)	(3.79)	(5.79)	(3.41)	(3.86)	
3.1E-02		4.70E-08	1.05E-05	1.02E-05	4.96E-08	2.46E-06	1.05E-05	1.00
(EOC)		(4.52)	(3.95)	(3.94)	(5.94)	(3.73)	(3.95)	
1.3E-01	5	2.69E-06	2.78E-04	2.60E-04	1.69E-05	4.39E-05	2.81E-04	1.01
6.3E-02		4.92E-08	9.98E-06	9.46E-06	1.53E-07	1.91E-06	9.80E-06	0.98
(EOC)		(5.77)	(4.80)	(4.78)	(6.78)	(4.53)	(4.84)	
3.1E-02		7.58E-10	3.22E-07	3.10E-07	1.77E-09	6.46E-08	3.18E-07	0.99
(EOC)		(6.02)	(4.95)	(4.93)	(6.44)	(4.88)	(4.94)	

Outline

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Quasi-linear elliptic problem

Quasi-linear elliptic problem

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

- quasi-linear diffusion problem

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

- Leray–Lions problem

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

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

Example

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

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

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

Weak formulation

Find $u \in V$ such that

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

Quasi-linear elliptic problem

Quasi-linear elliptic problem

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

- quasi-linear diffusion problem

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

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

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

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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

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

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

- 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

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

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- 1 Bibliography
- 2 Laplace equation
 - A guaranteed a posteriori error estimate
 - Polynomial-degree-robust local efficiency
 - Application and numerical results
- 3 **Quasi-linear elliptic problems**
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A posteriori error estimate

Assumption A (Total quasi-equilibrated flux reconstruction)

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

$$\nabla \cdot \sigma_h^{k,i} = f_h - \rho_h^{k,i},$$

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 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 $u_h^{k,i}$, $\sigma_h^{k,i}$, and $\rho_h^{k,i}$.

A posteriori error estimate

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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) $\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i} + \mathbf{a}_h^{k,i} = \boldsymbol{\sigma}_h^{k,i}$;
- (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
- $\mathbf{a}_h^{k,i}$: *algebraic error* flux reconstruction

Distinguishing error components

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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

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

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

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

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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

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

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 .

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Let the mesh \mathcal{T}_h be shape-regular and let the **local stopping criteria** hold. Then, under **Assumption C**,

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

for all $K \in \mathcal{T}_h$.

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

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Outline

- 1 Bibliography
- 2 Laplace equation
 - A guaranteed a posteriori error estimate
 - Polynomial-degree-robust local efficiency
 - Application and numerical results
- 3 Quasi-linear elliptic problems
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Application and numerical results
- 4 Two-phase flow in porous media
 - A guaranteed a posteriori error estimate
 - Applications and numerical results
- 5 Conclusions and future directions

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

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

- Do ν additional steps of the algebraic solver, yielding

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

- 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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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**

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

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Linearization

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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

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

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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

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Flux reconstructions

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

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

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

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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 $\sigma_h^{k,i} \in \mathbf{RTN}_0(\mathcal{S}_h)$.

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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

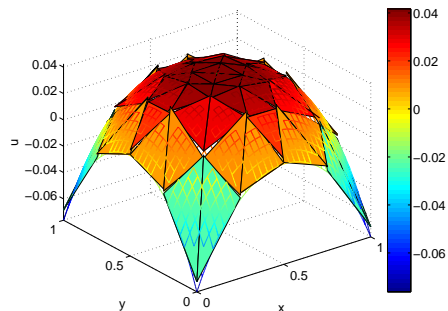
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_D && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

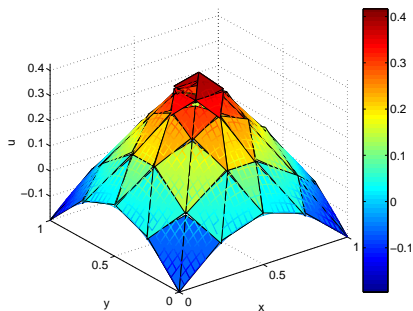
$$u(x, y) = -\frac{p-1}{p} \left(\left(x - \frac{1}{2}\right)^2 + \left(y - \frac{1}{2}\right)^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

Analytical and approximate solutions

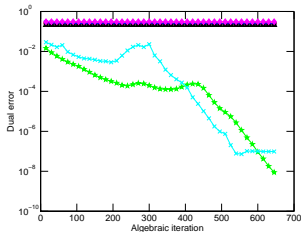


Case $p = 1.5$

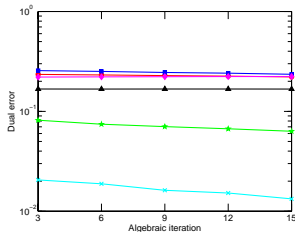


Case $p = 10$

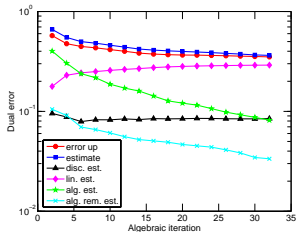
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

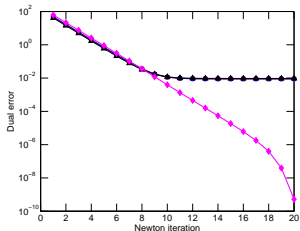


inexact Newton

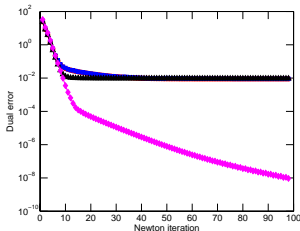


ad. inexact Newton

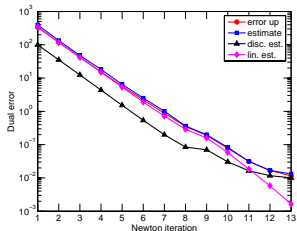
Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh



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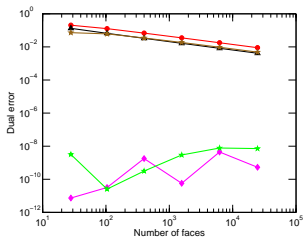


inexact Newton

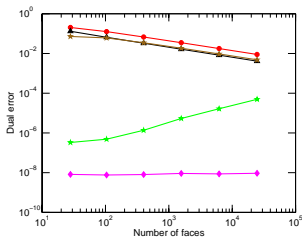


ad. inexact Newton

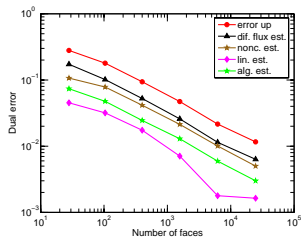
Error and estimators, $p = 10$



Newton

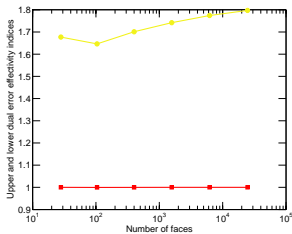


inexact Newton

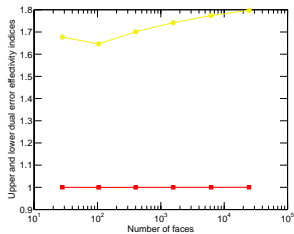


ad. inexact Newton

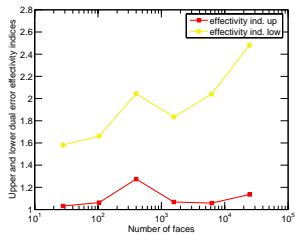
Effectivity indices, $p = 10$



Newton

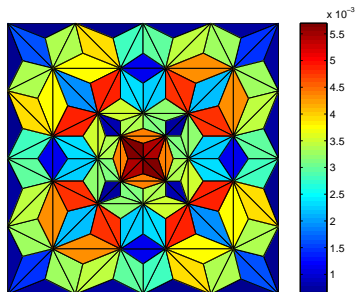


inexact Newton

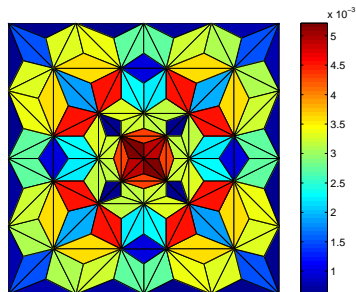


ad. inexact Newton

Error distribution, $p = 10$

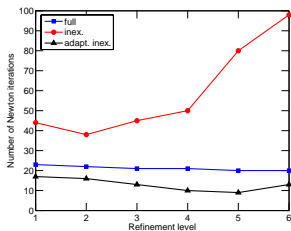


Estimated error distribution

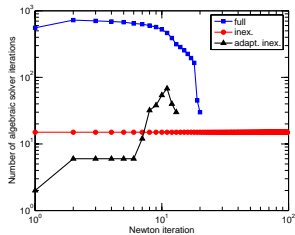


Exact error distribution

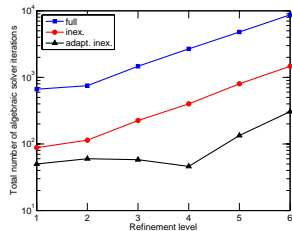
Newton and algebraic iterations, $p = 10$



Newton it. / refinement

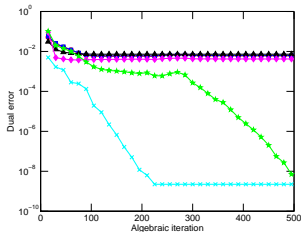


alg. it. / Newton step

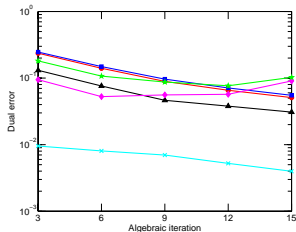


alg. it. / refinement

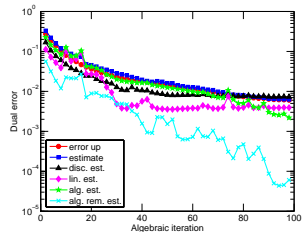
Error and estimators as a function of CG iterations, $\rho = 1.5$, 6th level mesh, 1st Newton step.



Newton

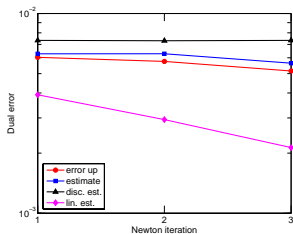
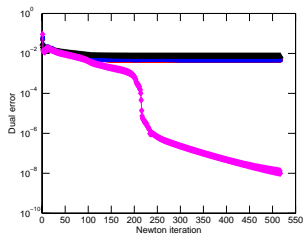
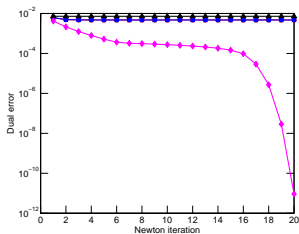


inexact Newton

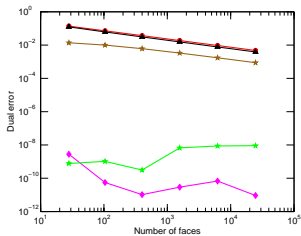


ad. inexact Newton

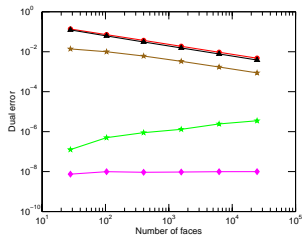
Error and estimators as a function of Newton iterations, $p = 1.5$, 6th level mesh



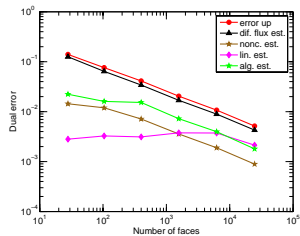
Error and estimators, $p = 1.5$



Newton

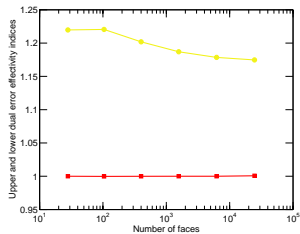


inexact Newton

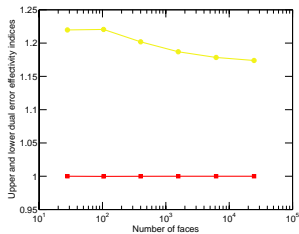


ad. inexact Newton

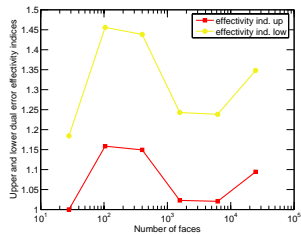
Effectivity indices, $p = 1.5$



Newton

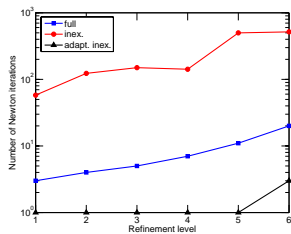


inexact Newton

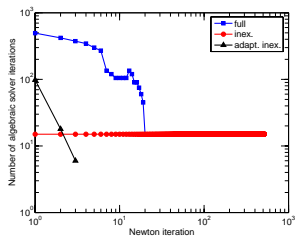


ad. inexact Newton

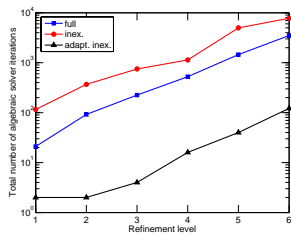
Newton and algebraic iterations, $p = 1.5$



Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p -Laplacian

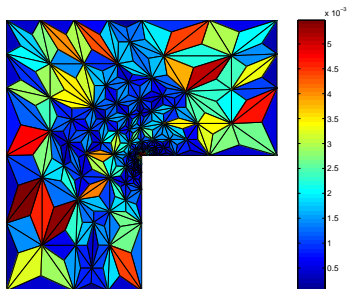
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_D && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

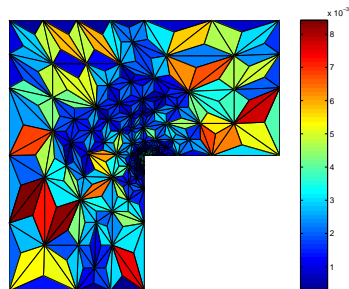
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

Error distribution on an adaptively refined mesh

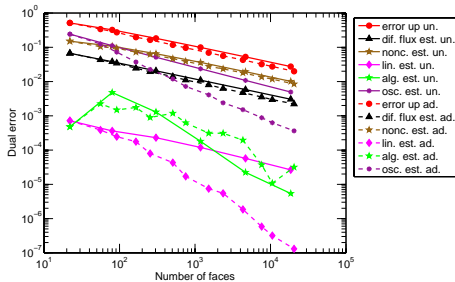


Estimated error distribution

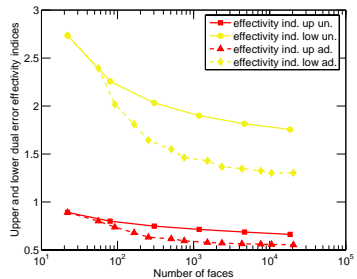


Exact error distribution

Estimated and actual errors and the effectivity index

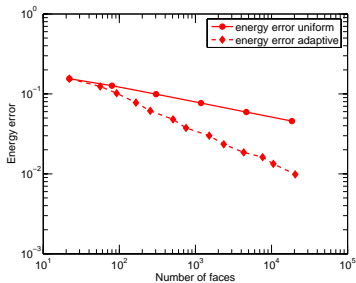


Estimated and actual errors

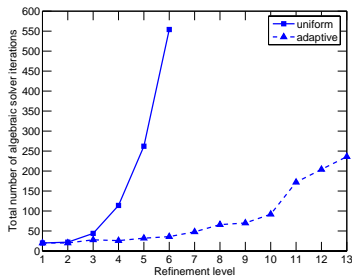


Effectivity index

Energy error and overall performance



Energy error



Overall performance

Outline

- 1 Bibliography
- 2 Laplace equation
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Two-phase flow in porous media

Two-phase flow in porous media

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

Mathematical issues

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

Two-phase flow in porous media

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Link energy-type error – dual norm of the residual

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

Let (s_w, p_w) be the **weak solution**. Let (s_{w,h_T}, p_{w,h_T}) be a vertex-centered finite volume / backward Euler approximation. Then

$$\begin{aligned} & \|s_w - s_{w,h_T}\|_{L^2((0,T);H^{-1}(\Omega))} + \|q(s_w) - q(s_{w,h_T})\|_{L^2(\Omega \times (0,T))} \\ & + \|p(s_w, p_w) - p(s_{w,h_T}, p_{w,h_T})\|_{L^2((0,T);H_0^1(\Omega))} \\ & \leq C \left\{ \sum_{n=1}^N \left\| (s_w - s_{w,h_T}, p_w - p_{w,h_T}) \right\|_{I_n}^2 \right\}^{\frac{1}{2}} \end{aligned}$$

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Distinguishing the error components

Theorem (Distinguishing the error components)

Let

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

with the approximations $(\mathbf{s}_{w,h_T}^{n,k,i}, \mathbf{p}_{w,h_T}^{n,k,i})$. Then

$$\|(\mathbf{s}_w - \mathbf{s}_{w,h_T}^{n,k,i}, \mathbf{p}_w - \mathbf{p}_{w,h_T}^{n,k,i})\|_n \leq \eta_{\text{sp}}^{n,k,i} + \eta_{\text{tm}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}.$$

Error components

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

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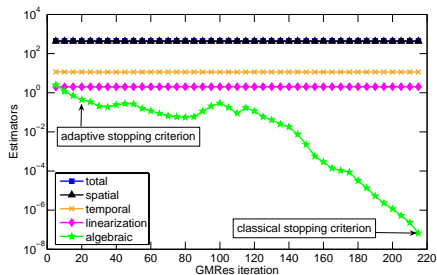
Error components

- $\eta_{sp}^{n,k,i}$: *spatial discretization*
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- $\eta_{lin}^{n,k,i}$: *linearization*
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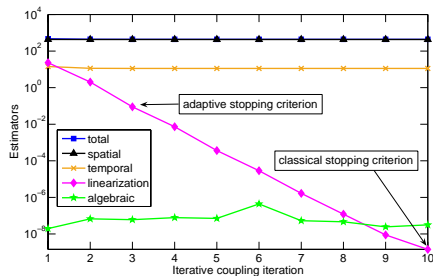
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- 2 Laplace equation
 - A guaranteed a posteriori error estimate
 - Polynomial-degree-robust local efficiency
 - Application and numerical results
- 3 Quasi-linear elliptic problems
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Estimators and stopping criteria

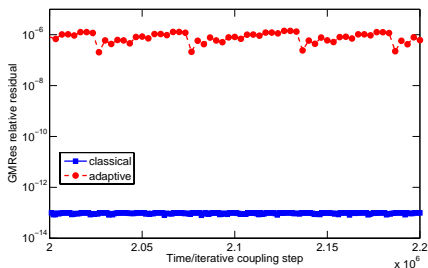


Estimators in function of
GMRes iterations

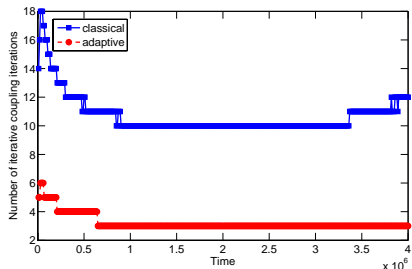


Estimators in function of
iterative coupling iterations

GMRes relative residual/iterative coupling iterations

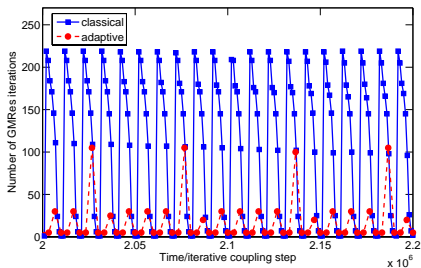


GMRes relative residual

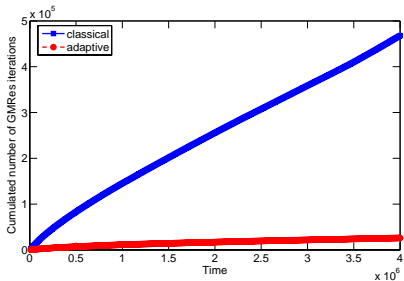


Iterative coupling iterations

GMRes iterations

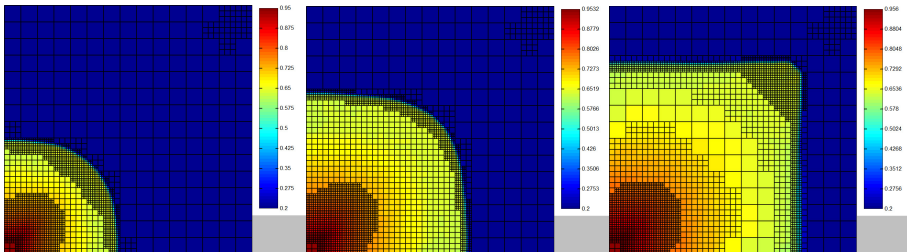


Per time and iterative
coupling step



Cumulated

Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

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- 2 Laplace equation
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Conclusions

Entire adaptivity

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

Future directions

- other coupled nonlinear systems
- convergence and optimality

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Bibliography

Bibliography

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- CANCÈS C., POP I. S., VOHRALÍK M., An a posteriori error estimate for vertex-centered finite volume discretizations of immiscible incompressible two-phase flow, *Math. Comp.* **83** (2014), 153–188.

Thank you for your attention!

