Adaptive inexact Newton methods

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Outline

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Inexact iterative linearization

System of nonlinear algebraic equations

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

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

Algorithm (Inexact iterative linearization)

1. *Choose initial vector U^0. Set $k := 1$.*
2. *$U^{k-1} \Rightarrow$ matrix $\mathbb{A}^{k-1}$ and vector F^{k-1}: find U^k s.t.*

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

3. 1. *Set $U^{k,0} := U^{k-1}$ and $i := 1$.*
   2. *Do an 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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Model steady problem, discretization

Quasi-linear elliptic problem

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

- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$
- example: p-Laplacian with $\boldsymbol{\sigma}(u,\nabla u) = |\nabla u|^{p-2}\nabla u$
- f piecewise polynomial for simplicity
- weak solution: $u \in V := W_0^{1,p}(\Omega)$ such that

$$(\boldsymbol{\sigma}(u,\nabla u),\nabla v) = (f,v) \qquad \forall v \in V$$

Numerical approximation

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

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Intrinsic error measure

Energy error in the Laplace case

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

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$$+ \underbrace{\left\{ \sum_{K \in \mathcal{T}_h} \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u - u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}}}_{\text{distance of } u_h \text{ to } V}$$

- there holds $\mathcal{J}_u(u_h^{k,i}) = 0$ if and only if $u = u_h^{k,i}$

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Abstract assumptions

Assumption A (Total flux reconstruction)

There exists $\boldsymbol{\sigma}_h^{k,i} \in \mathbf{H}^q(\mathrm{div},\Omega)$ *and* $\rho_h^{k,i} \in L^q(\Omega)$ *such that*

$$\nabla\cdot\boldsymbol{\sigma}_h^{k,i} = f - \underbrace{\rho_h^{k,i}}_{\text{algebraic remainder}}.$$

Assumption B (Discretization, linearization, and alg. fluxes)

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

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

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

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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

$$\mathcal{J}_u(u_h^{k,i}) \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i}.$$

Estimators

- *discretization* estimator

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

- *linearization* estimator

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

- *algebraic* estimator

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

- *algebraic remainder estimator*

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

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

Outline

Stopping criteria

Global stopping criteria

- stop whenever:

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

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

Local stopping criteria

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

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

Assumptions for efficiency

Assumption C (Piecewise polynomials, meshes, quadrature)

The approximation $u_h^{k,i}$ is piecewise polynomial. The meshes $\mathcal{T}_h$ are shape-regular. The quadrature error is negligible.

Assumption D (Approximation property)

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

$$\|\sigma(u_h^{k,i}, \nabla u_h^{k,i}) + \mathbf{d}_h^{k,i}\|_{q,K} \le C \left\{ \sum_{K' \in \mathfrak{T}_K} h_{K'}^q \|f + \nabla\cdot\sigma(u_h^{k,i}, \nabla u_h^{k,i})\|_{q,K'}^q + \sum_{e \in \mathfrak{E}_K^{\mathrm{int}}} h_e \|[\![\sigma(u_h^{k,i}, \nabla u_h^{k,i})\cdot\mathbf{n}_e]\!]\|_{q,e}^q + \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[\![u_h^{k,i}]\!]\|_{q,e}^q \right\}^{\frac{1}{q}}.$$

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Global efficiency

Theorem (Global efficiency)

Let the Assumptions C and D be satisfied. Let the global stopping criteria hold. Then,

$$\eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i} \leq C \mathcal{J}_u(u_h^{k,i}),$$

where C is independent of σ and q.

Theorem (Local efficiency)

Let the Assumptions C and D be satisfied. Let the ***local*** *stopping criteria hold. Then*

$$\eta_{\mathrm{disc},K}^{k,i} + \eta_{\mathrm{lin},K}^{k,i} + \eta_{\mathrm{alg},K}^{k,i} + \eta_{\mathrm{rem},K}^{k,i} \leq C \mathcal{J}_{u,\mathfrak{T}_K}(u_h^{k,i}) \qquad \forall K \in \mathcal{T}_h.$$

- **robustness** with respect to the **nonlinearity** thanks to the choice of $\mathcal{J}_u$ as error measure

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$$\eta_{\mathrm{disc},K}^{k,i} + \eta_{\mathrm{lin},K}^{k,i} + \eta_{\mathrm{alg},K}^{k,i} + \eta_{\mathrm{rem},K}^{k,i} \le C \mathcal{J}_{u,\mathfrak{T}_K}(u_h^{k,i}) \qquad \forall K \in \mathcal{T}_h.$$

- **robustness** with respect to the **nonlinearity** thanks to the choice of $\mathcal{J}_u$ as error measure

Global efficiency

Theorem (Global efficiency)

Let the Assumptions C and D be satisfied. Let the global stopping criteria hold. Then,

$$\eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i} \leq C \mathcal{J}_u(u_h^{k,i}),$$

where C is independent of σ and q.

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Outline

Nonconforming finite elements for the p-Laplacian

Discretization

Find $u_h \in V_h$ such that

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

- $\sigma(\nabla u_h) = |\nabla u_h|^{p-2}\nabla u_h$
- $V_h \not\subset V$ the Crouzeix–Raviart space
- leads to the system of nonlinear algebraic equations

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Linearization

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Find $u_h^k \in V_h$ such that

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

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

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

- Newton linearization

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

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Algebraic solution

Algebraic solution

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

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

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

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Flux reconstructions

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

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

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

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Set $\mathbf{a}_h^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i})$ for (adaptively chosen) $\nu > 0$ additional algebraic solvers steps; $R^{k,i+\nu} \rightsquigarrow \rho_h^{k,i}$.

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Verification of the assumptions

Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

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

Lemma (Assumptions C and D)

Assumptions C and D hold.

Comments

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

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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 D verified

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Outline

Numerical experiment I

Model problem

- p-Laplacian

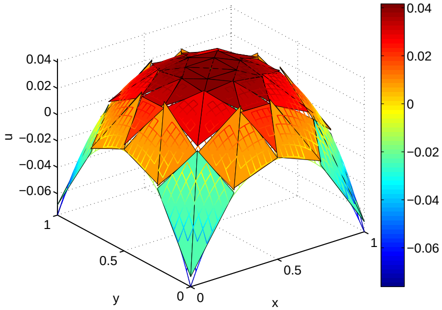
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

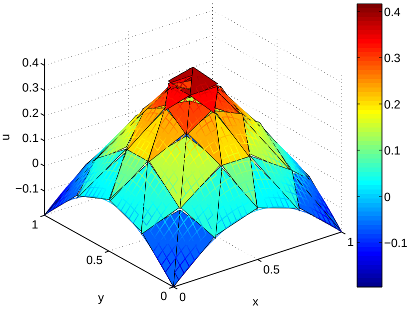
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2+(y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

Analytical and approximate solutions

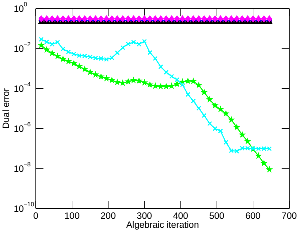


Case $p = 1.5$

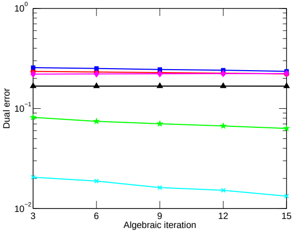


Case $p = 10$

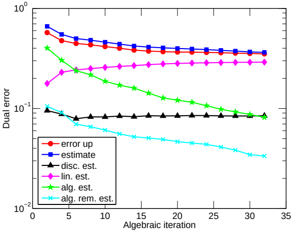
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

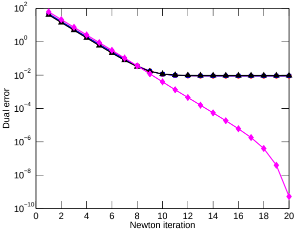


inexact Newton

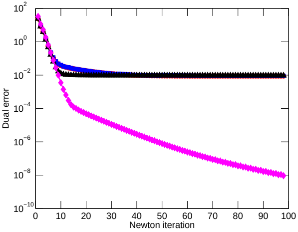


ad. inexact Newton

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



Newton



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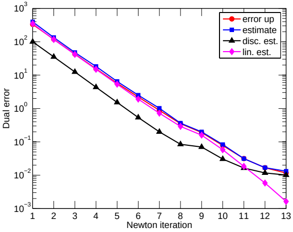
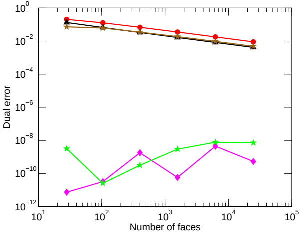
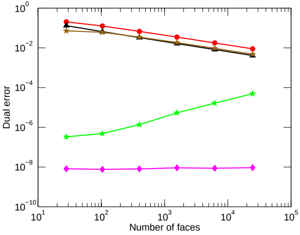


ad. inexact Newton

Error and estimators, $p = 10$



Newton



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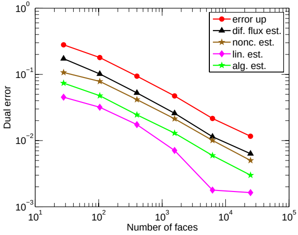
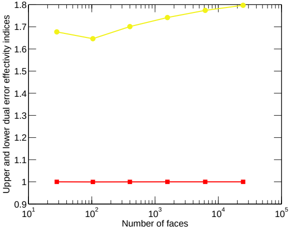
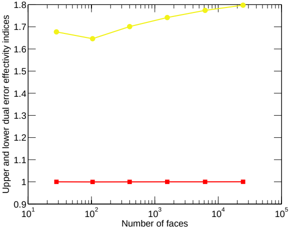


ad. inexact Newton

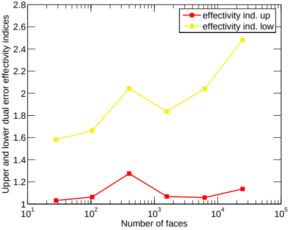
Effectivity indices, $p = 10$



Newton

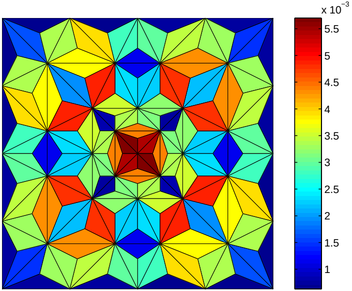


inexact Newton

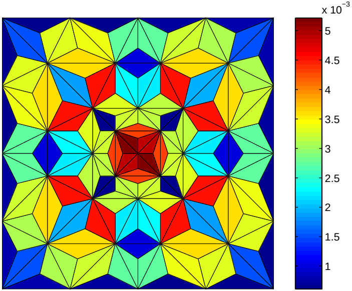


ad. inexact Newton

Error distribution, $p = 10$

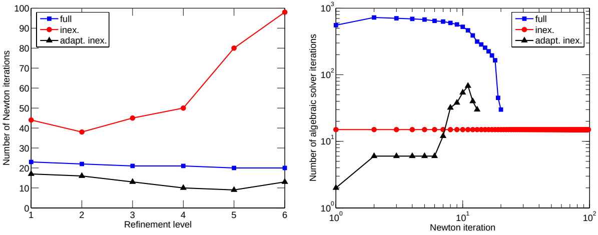


Estimated error distribution



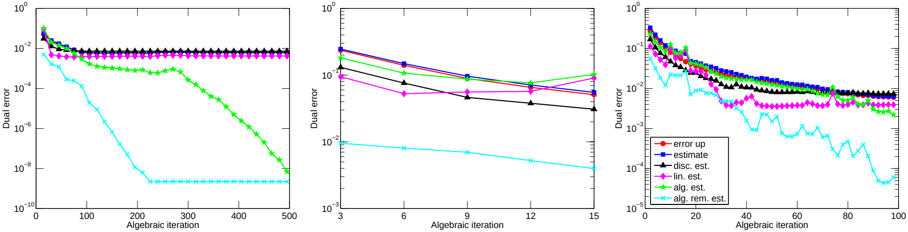
Exact error distribution

Newton and algebraic iterations, $p = 10$



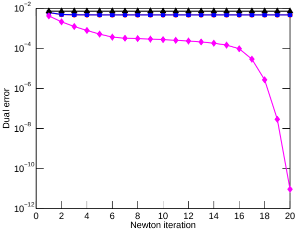
Newton it. / refinement   alg. it. / Newton step   alg. it. / refinement

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

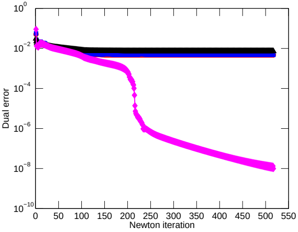


Newton | inexact Newton | ad. inexact Newton

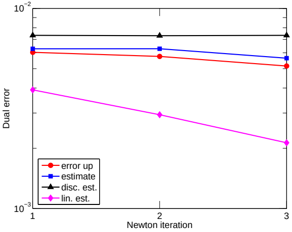
Error and estimators as a function of Newton iterations, $p = 1.5$, 6th level mesh



Newton



inexact Newton



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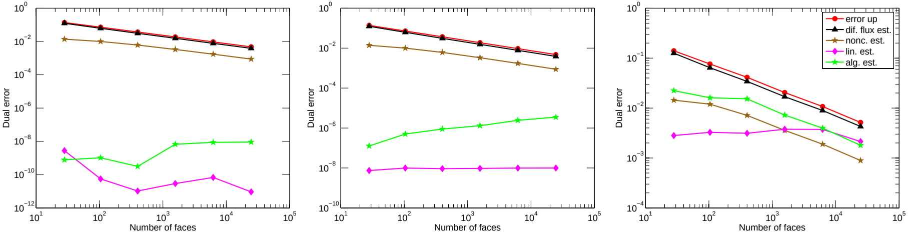
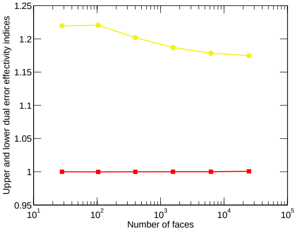


Newton inexact Newton ad. inexact Newton

Effectivity indices, $p = 1.5$



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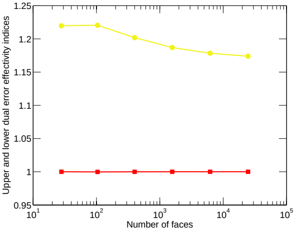
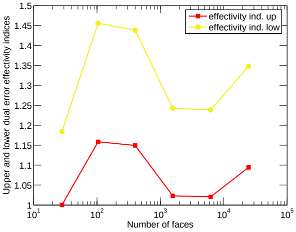


inexact Newton



ad. inexact Newton

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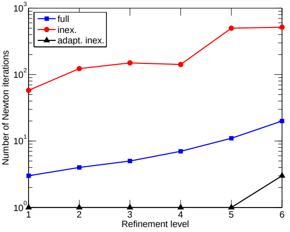
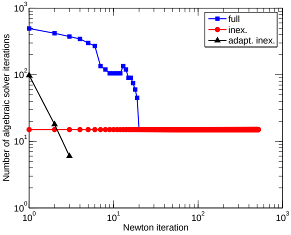
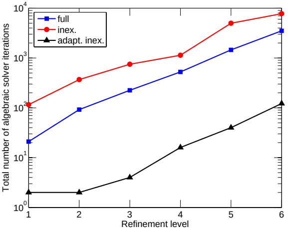


Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p-Laplacian

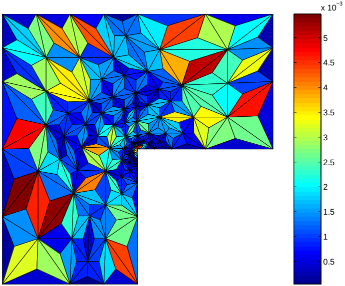
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

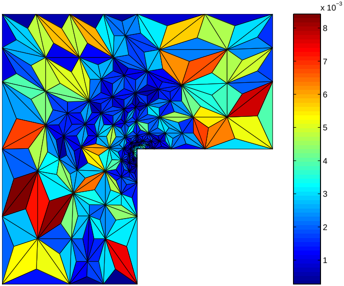
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

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

Error distribution on an adaptively refined mesh

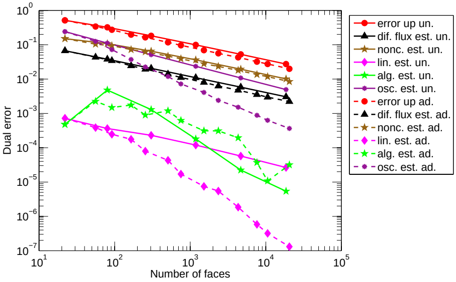


Estimated error distribution

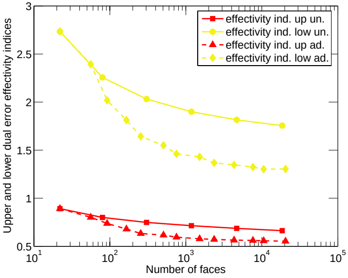


Exact error distribution

Estimated and actual errors and the effectivity index

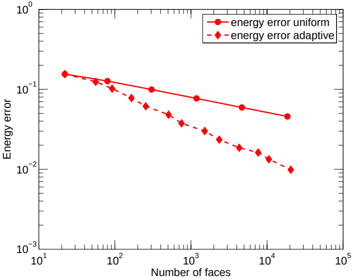


Estimated and actual errors

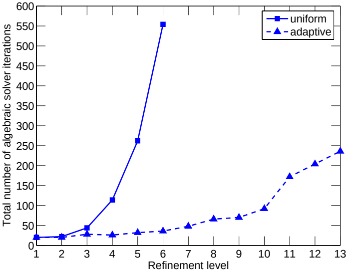


Effectivity index

Energy error and overall performance



Energy error



Overall performance

Outline

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
- Deuflhard (1990's, 2004 book), adaptivity

Stopping criteria for algebraic solvers

- engineering literature, since 1950's
- Becker, Johnson, and Rannacher (1995), multigrid stopping criterion
- Arioli (2000's), comparison of the algebraic and discretization errors

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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

Bibliography

Bibliography

- Ern A., Vohralík M., Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs, *SIAM J. Sci. Comput.* **35** (2013), A1761–A1791.

Thank you for your attention!