

Flux and potential reconstructions  
for guaranteed error bounds  
in numerical approximations of model PDEs

**Martin Vohralík**

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# Outline

- 1 Introduction
- 2 Laplace equation: potential & flux reconstructions
  - Guaranteed upper bound in a unified framework
  - Polynomial-degree-robust local efficiency
  - Applications & numerical results
- 3 Nonlinear Laplace equation: adaptive stopping criteria
  - Adaptive inexact Newton method
  - Applications & numerical results
- 4 Laplace eigenvalues and eigenvectors: guaranteed bounds
  - Applications & numerical results
- 5 Heat equation: robustness wrt final time & local efficiency
- 6 Two-phase flow in porous media: industrial application
- 7 Conclusions and outlook

# Optimal a posteriori error estimate

## Guaranteed upper bound

- $\|u - u_h\|_{?,\Omega}^2 \leq \sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2$
- no undetermined constant: **error control**

## Local efficiency

- $\eta_K(u_h) \leq C_{\text{eff}} \|u - u_h\|_{?, \text{neighbors of } K}$
- **local** error lower bound (optimal space mesh refinement)

## Robustness

- $C_{\text{eff}}$  independent of data, domain  $\Omega$ , meshes, solution  $u$ , **polynomial degree** of  $u_h$

## Asymptotic exactness

- $\sum_{K \in \mathcal{T}_h} \eta_K(u_h)^2 / \|u - u_h\|_{?,\Omega}^2 \searrow 1$
- overestimation factor goes to one with meshes size

## Small evaluation cost

- estimators  $\eta_K(u_h)$  can be evaluated cheaply (locally)

## Error components identification

- $\eta_K(u_h)$  can distinguish the different error components

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# Laplace model problem

## Model problem

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega \end{aligned}$$

- $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$  polygon/polyhedron
- $f \in L^2(\Omega)$

## Weak formulation

Find  $u \in H_0^1(\Omega)$  such that

$$(\nabla u, \nabla v) = (f, v) \quad \forall v \in H_0^1(\Omega)$$

## Properties of the weak solution

- $u \in H_0^1(\Omega)$  (primal variable constraint)
- $\sigma := -\nabla u$  (constitutive relation)
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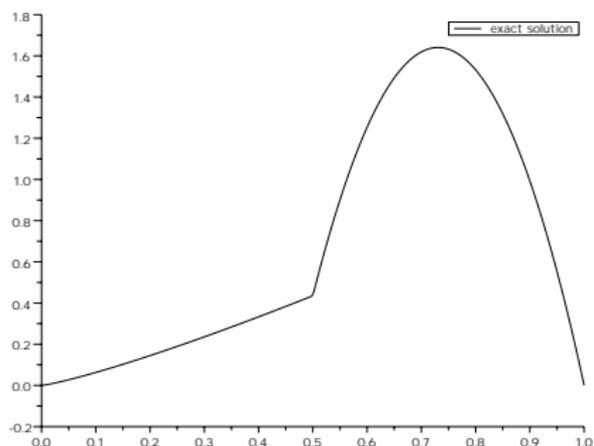
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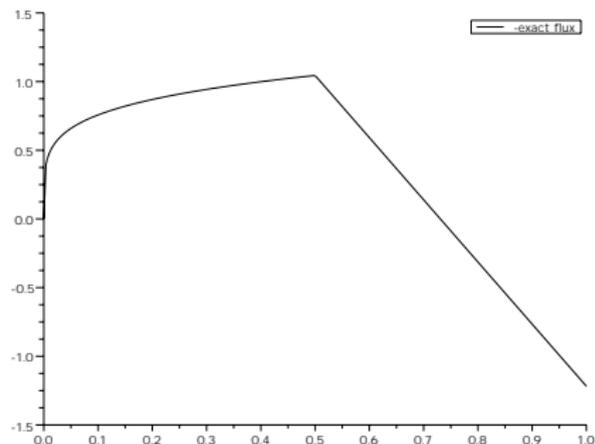
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# Exact solution and flux

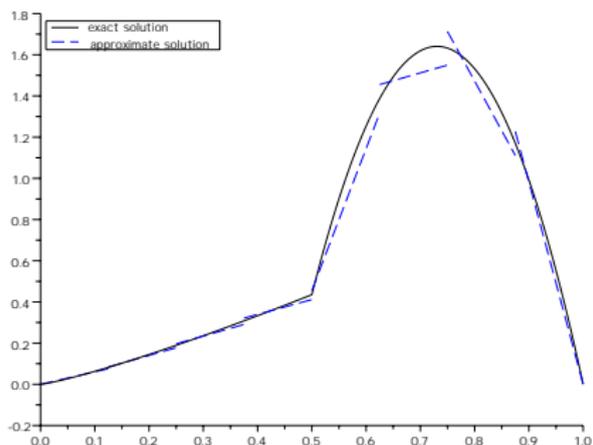


Solution  $u$  is continuous

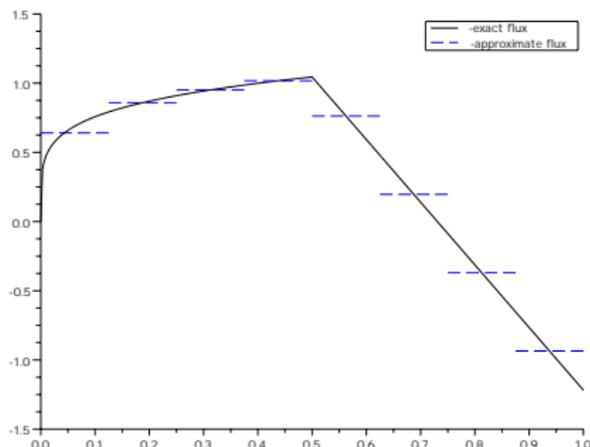


Flux  $\sigma := -\underline{K}\nabla u$  is continuous

# Approximate solution and flux

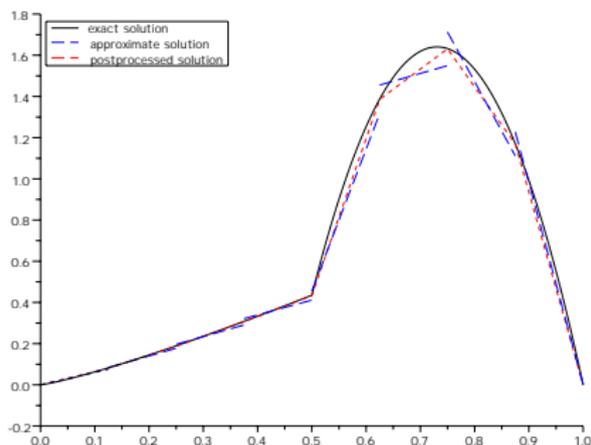


Approximate solution  $u_h$  is **not** necessarily continuous

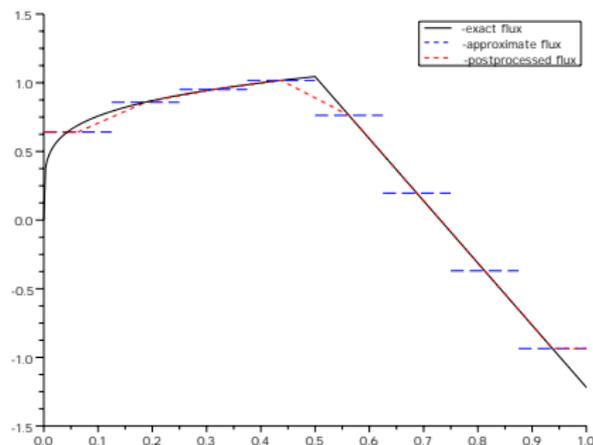


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# Potential and flux reconstructions



Potential reconstruction



Flux reconstruction

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**Theorem (A guaranteed a posteriori error estimate, Prager and Synge (1947), Ladevèze (1975), Dari, Durán, Padra, & Vampa (1996), Ainsworth (2005), Kim (2007), Vohralík (2007), ...)**

- 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  $\sigma_h \in \mathbf{H}(\text{div}, \Omega)$  be such that

$$(\nabla \cdot \sigma_h, 1)_K = (f, 1)_K \text{ for all } K \in \mathcal{T}_h.$$

Then

$$\begin{aligned} \|\nabla(u - u_h)\|^2 \leq & \sum_{K \in \mathcal{T}_h} \left( \underbrace{\|\nabla u_h + \sigma_h\|_K}_{\text{constitutive relation}} + \underbrace{\frac{h_K}{\pi} \|f - \nabla \cdot \sigma_h\|_K}_{\text{equilibrium}} \right)^2 \\ & + \sum_{K \in \mathcal{T}_h} \underbrace{\|\nabla(u_h - s_h)\|_K^2}_{\text{primal constraint}}. \end{aligned}$$

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- 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)

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

- projection definition of  $s$ :

$$\|\nabla(s - u_h)\| = \underbrace{\min_{v \in H_0^1(\Omega)} \|\nabla(v - u_h)\|}_{\text{distance of } u_h \text{ to } H_0^1(\Omega)}$$

- dual norm characterization definition of  $s$ , definition of  $u$ :

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# Proof II

## Proof (continuation).

- nonconformity upper bound:

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

- adding and subtracting equilibrated flux, Green theorem:

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

- Cauchy–Schwarz and Poincaré inequalities, equilibration:

$$- (\nabla u_h + \sigma_h, \nabla \varphi)$$

$$(f - \nabla \cdot \sigma_h, \varphi) = \sum_{K \in \mathcal{T}_h} (f - \nabla \cdot \sigma_h, \varphi)_K$$

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

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# Global potential and flux reconstructions

## Ideally

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

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

- ✓ computable, discrete spaces  $V_h \subset H_0^1(\Omega)$ ,  $\mathbf{V}_h \subset \mathbf{H}(\text{div}, \Omega)$ ,  $Q_h \subset L^2(\Omega)$
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# Local potential reconstruction

Definition (Construction of  $s_h$ ,  $\approx$  Carstensen and Merdon (2013), EV (2015))

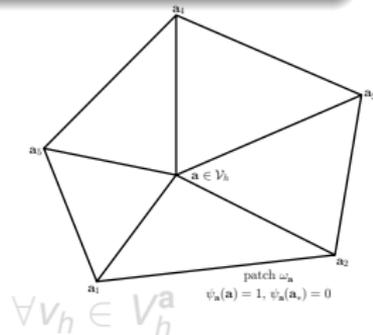
For each  $\mathbf{a} \in \mathcal{V}_h$ , solve the **local conforming FE problem**

$$s_h^{\mathbf{a}} := \arg \min_{v_h \in V_h^{\mathbf{a}}} \|\nabla(\psi_{\mathbf{a}} u_h - v_h)\|_{\omega_{\mathbf{a}}}.$$

## Equivalent form

Find  $s_h^{\mathbf{a}} \in V_h^{\mathbf{a}}$  such that

$$(\nabla s_h^{\mathbf{a}}, \nabla v_h)_{\omega_{\mathbf{a}}} = (\nabla(\psi_{\mathbf{a}} u_h), \nabla v_h)_{\omega_{\mathbf{a}}}$$



$$\forall v_h \in V_h^{\mathbf{a}}$$

## Key ideas

- **local minimizations**
- **cut-off** by hat basis functions  $\psi_{\mathbf{a}}$
- $V_h^{\mathbf{a}} \subset H_0^1(\omega_{\mathbf{a}})$ : homogeneous **Dirichlet** BC on  $\partial\omega_{\mathbf{a}}$
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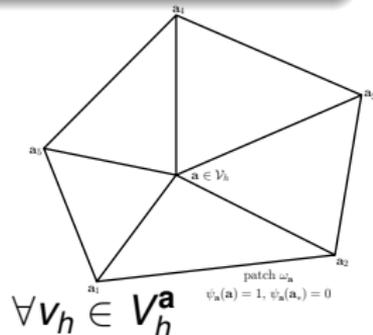
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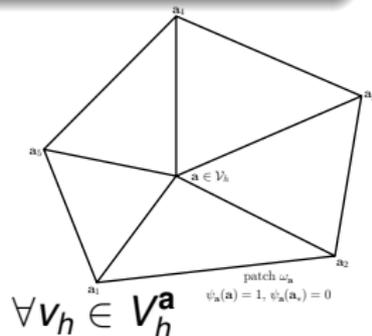
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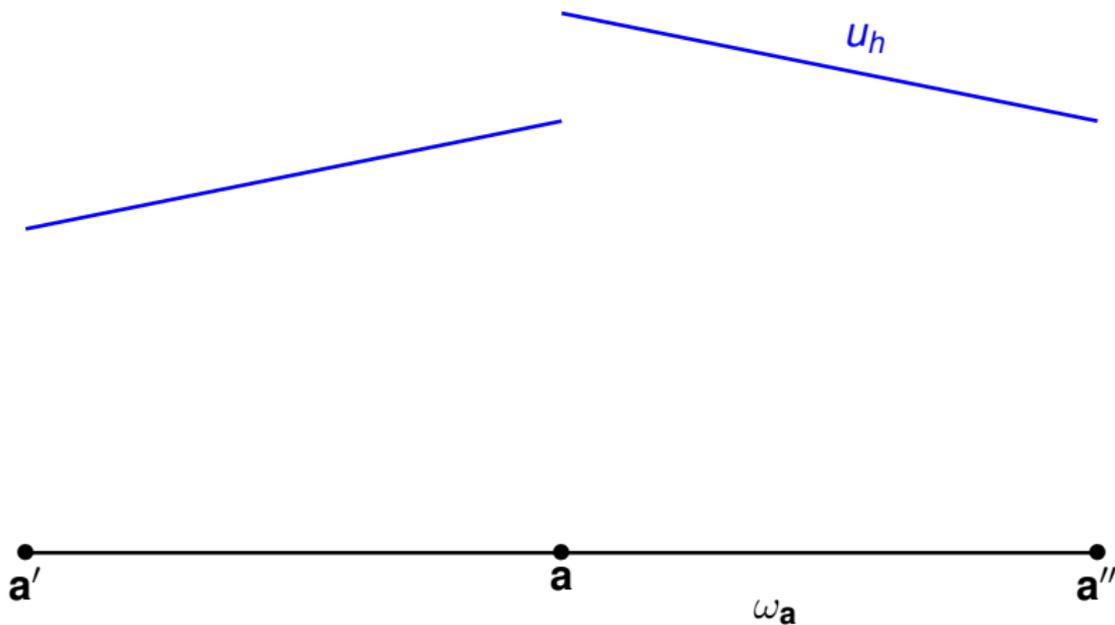
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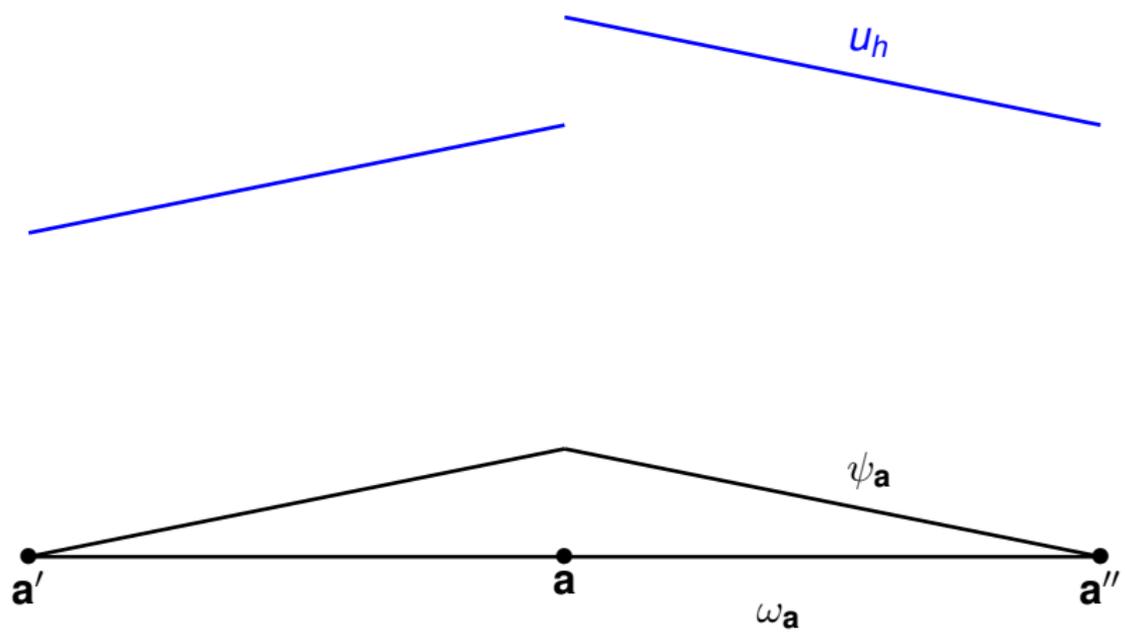
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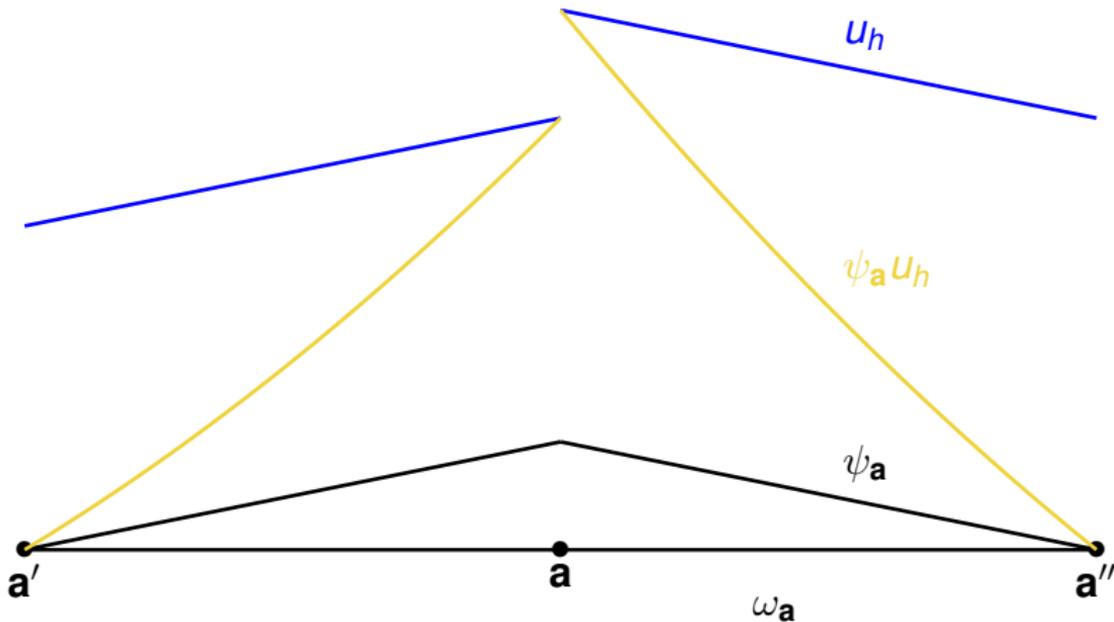
# Potential reconstruction in 1D



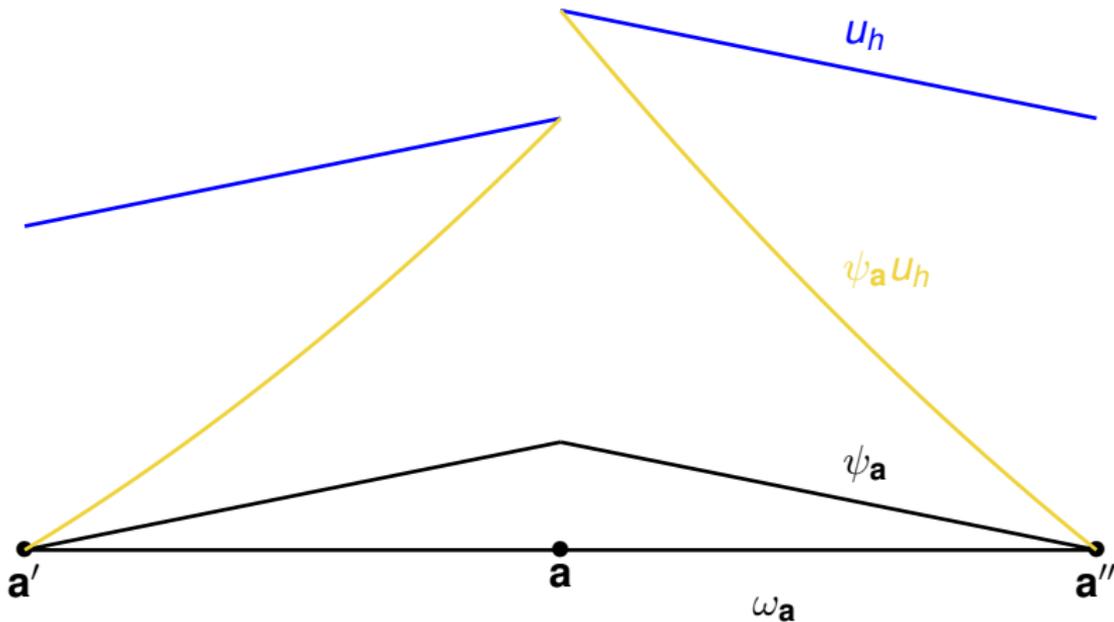
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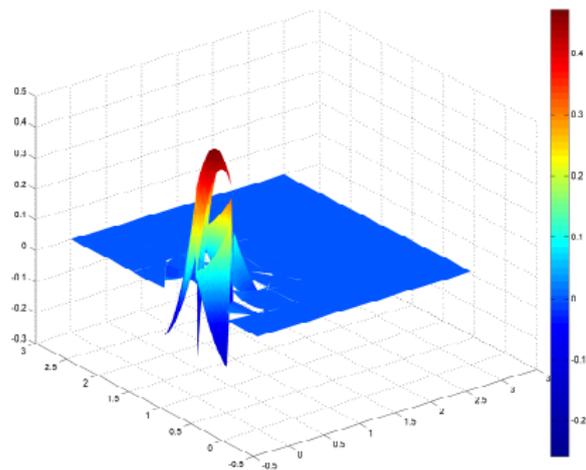
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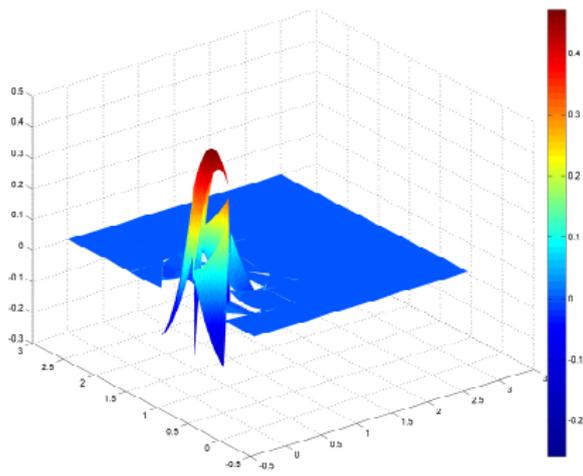


# Potential reconstruction in 2D

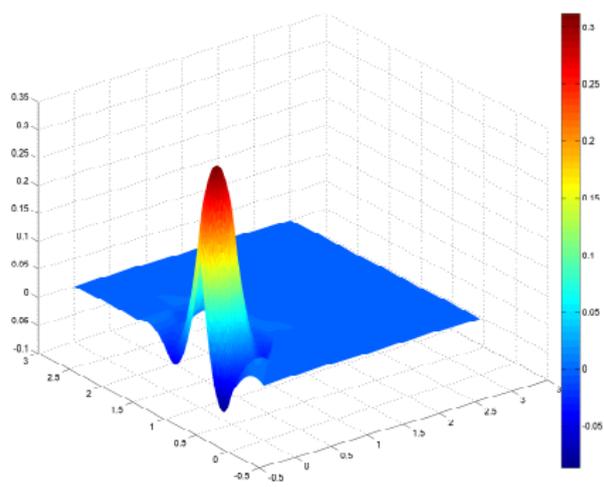


Potential  $u_h$

# Potential reconstruction in 2D



Potential  $u_h$



Potential reconstruction  $s_h$

# Local flux reconstructions

## Assumption A (Galerkin orthogonality wrt hat functions)

There holds

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

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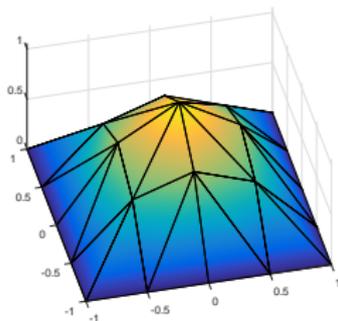
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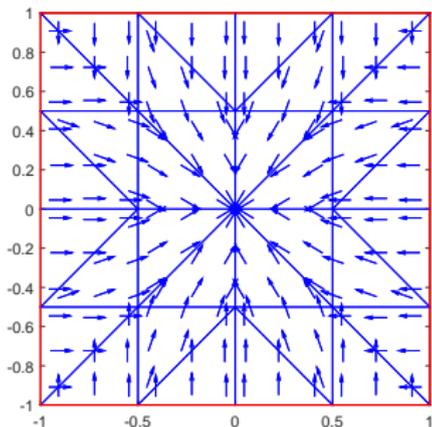
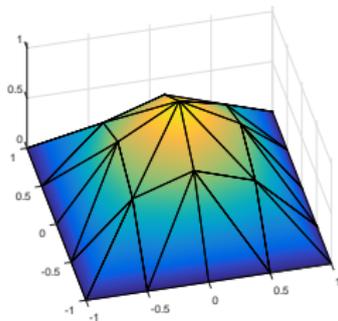
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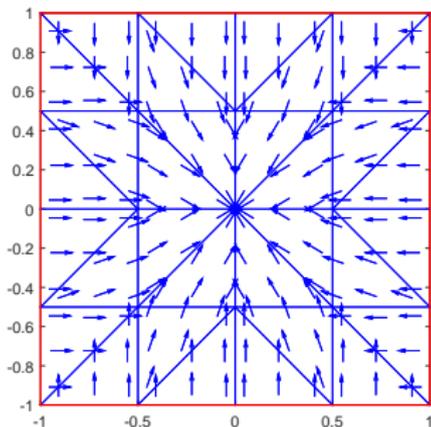
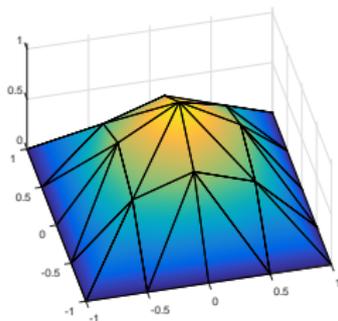


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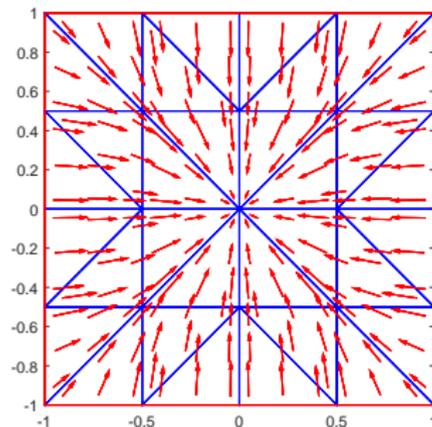


Flux  $-\nabla u_h$

# Equilibrated flux reconstruction



Flux  $-\nabla u_h$



Flux reconstruction  $\sigma_h$

# Outline

- 1 Introduction
- 2 Laplace equation: potential & flux reconstructions
  - Guaranteed upper bound in a unified framework
  - Polynomial-degree-robust local efficiency
  - Applications & numerical results
- 3 Nonlinear Laplace equation: adaptive stopping criteria
  - Adaptive inexact Newton method
  - Applications & numerical results
- 4 Laplace eigenvalues and eigenvectors: guaranteed bounds
  - Applications & numerical results
- 5 Heat equation: robustness wrt final time & local efficiency
- 6 Two-phase flow in porous media: industrial application
- 7 Conclusions and outlook

# Polynomial-degree-robust efficiency

## Assumption B (Piecewise polynomials, data, and meshes)

The approximation  $u_h$  and the datum  $f$  are *piecewise polynomial*. The *degrees* of the MFE reconstructions  $\sigma_h$  and  $s_h$  are chosen correspondingly. The meshes  $\mathcal{T}_h$  are *shape-regular*.

Theorem (Polynomial-degree-robust efficiency Braess, Pillwein, and Schöberl (2009); Costabel and McIntosh (2010); Demkowicz, Gopalakrishnan, and Schöberl (2012), EV (2015))

Let  $u$  be the weak solution and let *Assumptions A and B* hold. Then there exists constants  $C_{\text{st}}, C_{\text{cont,PF}}, C_{\text{cont,bPF}} > 0$  *only depending* on the shape-regularity parameter  $\kappa_{\mathcal{T}}$  such that

$$\begin{aligned} \|\sigma_h^a + \psi_a \nabla u_h\|_{\omega_a} &\leq C_{\text{st}} C_{\text{cont,PF}} \|\nabla(u - u_h)\|_{\omega_a}, \\ \|\nabla(\psi_a u_h - s_h^a)\|_{\omega_a} &\leq C_{\text{st}} C_{\text{cont,bPF}} \|\nabla(u - u_h)\|_{\omega_a} + \text{jumps}. \end{aligned}$$

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# Potentials (Demkowicz, Gopalakrishnan, Schöberl (2009), EV 2016)

Lemma ( $H^1$  polynomial extension on a tetrahedron)

Let  $K \in \mathcal{T}_h$ ,  $\mathcal{E}_K^D \subset \mathcal{E}_K$ . Let  $r \in \mathbb{P}_p(\mathcal{E}_K^D)$  be continuous on  $\mathcal{E}_K^D$ . Then for  $C$  only depending on the shape regularity of  $K$ ,

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## Context

$$\begin{aligned} -\Delta \zeta_K &= 0 && \text{in } K, \\ \zeta_K &= r_e && \text{on all } e \in \mathcal{E}_K^D, \\ -\nabla \zeta_K \cdot \mathbf{n}_K &= 0 && \text{on all } e \in \mathcal{E}_K \setminus \mathcal{E}_K^D. \end{aligned}$$

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$$\min_{\substack{v_h \in \mathbb{P}_p(K) \\ v_h = r_e \text{ on all } e \in \mathcal{E}_K^D}} \|\nabla v_h\|_K \leq C \underbrace{\min_{\substack{v \in H^1(K) \\ v = r_e \text{ on all } e \in \mathcal{E}_K^D}} \|\nabla v\|_K}_{\|r\|_{H^{1/2}(\partial K)}} = C \|\nabla \zeta_K\|_K.$$

## Context

$$\begin{aligned} -\Delta \zeta_K &= 0 && \text{in } K, \\ \zeta_K &= r_e && \text{on all } e \in \mathcal{E}_K^D, \\ -\nabla \zeta_K \cdot \mathbf{n}_K &= 0 && \text{on all } e \in \mathcal{E}_K \setminus \mathcal{E}_K^D. \end{aligned}$$

# Potentials (Demkowicz, Gopalakrishnan, Schöberl (2009), EV 2016)

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# Fluxes (Costabel, McIntosh (2010), Demkowicz, Gopalakrishnan, Schöberl (2012), EV 2016)

## Lemma ( $\mathbf{H}(\text{div})$ polynomial extension on a tetrahedron)

Let  $K \in \mathcal{T}_h$ ,  $\mathcal{E}_K^N \subset \mathcal{E}_K$ . Let  $r \in \mathbb{P}_p(\mathcal{E}_K^N) \times \mathbb{P}_p(K)$ , satisfying  $\sum_{e \in \mathcal{E}_K} (r_e, 1)_e = (r_K, 1)_K$  if  $\mathcal{E}_K^N = \mathcal{E}_K$ . Then for  $C = C(\kappa_K) > 0$ ,

$$\min_{\substack{\mathbf{v}_h \in \mathbf{RTN}_p(K) \\ \mathbf{v}_h \cdot \mathbf{n}_K = r_e \quad \forall e \in \mathcal{E}_K^N \\ \nabla \cdot \mathbf{v}_h = r_K}} \|\mathbf{v}_h\|_K \leq C \min_{\substack{\mathbf{v} \in \mathbf{H}(\text{div}, K) \\ \mathbf{v} \cdot \mathbf{n}_K = r_e \quad \forall e \in \mathcal{E}_K^N \\ \nabla \cdot \mathbf{v} = r_K}} \|\mathbf{v}\|_K .$$

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# Outline

- 1 Introduction
- 2 Laplace equation: potential & flux reconstructions
  - Guaranteed upper bound in a unified framework
  - Polynomial-degree-robust local efficiency
  - **Applications & numerical results**
- 3 Nonlinear Laplace equation: adaptive stopping criteria
  - Adaptive inexact Newton method
  - Applications & numerical results
- 4 Laplace eigenvalues and eigenvectors: guaranteed bounds
  - Applications & numerical results
- 5 Heat equation: robustness wrt final time & local efficiency
- 6 Two-phase flow in porous media: industrial application
- 7 Conclusions and outlook

# Conforming finite elements

## Conforming finite elements

Find  $u_h \in V_h$  such that

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

- $V_h := \mathbb{P}_\rho(\mathcal{T}_h) \cap H_0^1(\Omega)$ ,  $\rho \geq 1$
- ✓ Assumption A: take  $v_h = \psi_a$
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Find  $u_h \in V_h$  such that

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

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$$\nabla_d u_h := \nabla u_h - \theta \sum_{e \in \mathcal{E}_h} l_e([u_h])$$

- jumps lifting operator  $l_e : L^2(e) \rightarrow [\mathbb{P}_0(\mathcal{T}_e)]^2$ 

$$(l_e([u_h]), \mathbf{v}_h) = \langle \{\{\mathbf{v}_h\}\} \cdot \mathbf{n}_e, [u_h] \rangle_e \quad \forall \mathbf{v}_h \in [\mathbb{P}_0(\mathcal{T}_e)]^2$$
- $\Rightarrow$  modified Galerkin orthogonality

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

# Numerics: smooth case

## Model problem

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega &:= (0, 1)^2, \\ u &= 0 & \text{on } \partial\Omega \end{aligned}$$

## Exact solution

$$u(x, y) = \sin(2\pi x) \sin(2\pi y)$$

## Discretization

- symmetric interior penalty discontinuous Galerkin method
- unstructured triangular grids
- uniform  $h$  refinement

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# Uniform refinement: asymptotic exactness

$h$	$p$	$\ \nabla_d(u - u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	$\eta_{\text{osc}}$	$\ \nabla_d(u_h - s_h)\ $	$\eta$	$\rho^{\text{eff}}$
$h_0$	<b>1</b>	1.07E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	<b>1.17</b>
$\approx h_0/2$		5.56E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	<b>1.09</b>
$\approx h_0/4$		2.92E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	<b>1.06</b>
$\approx h_0/8$		1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	<b>1.04</b>
$h_0$	<b>2</b>	1.54E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	<b>1.06</b>
$\approx h_0/2$		4.07E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	<b>1.04</b>
$\approx h_0/4$		1.10E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	<b>1.03</b>
$\approx h_0/8$		2.50E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	<b>1.03</b>
$h_0$	<b>3</b>	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	<b>1.03</b>
$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	<b>1.01</b>
$\approx h_0/4$		2.60E-04	2.60E-04	4.73E-07	2.54E-05	2.62E-04	<b>1.01</b>
$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	<b>1.01</b>
$h_0$	<b>4</b>	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	<b>1.02</b>
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	<b>1.01</b>
$\approx h_0/4$		5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	<b>1.01</b>
$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	<b>1.01</b>
$h_0$	<b>5</b>	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	<b>1.02</b>
$\approx h_0/2$		2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	<b>1.01</b>
$\approx h_0/4$		7.74E-08	7.73E-08	1.01E-10	4.35E-09	7.76E-08	<b>1.00</b>
$\approx h_0/8$		1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	<b>1.00</b>
$h_0$	<b>6</b>	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	<b>1.02</b>
$\approx h_0/2$		5.42E-08	5.42E-08	2.40E-10	4.02E-09	5.46E-08	<b>1.01</b>
$\approx h_0/4$		1.07E-09	1.07E-09	1.03E-11	6.90E-11	1.08E-09	<b>1.01</b>

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$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	<b>1.01</b>
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$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	<b>1.01</b>
$h_0$	<b>4</b>	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	<b>1.02</b>
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	<b>1.01</b>
$\approx h_0/4$		5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	<b>1.01</b>
$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	<b>1.01</b>
$h_0$	<b>5</b>	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	<b>1.02</b>
$\approx h_0/2$		2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	<b>1.01</b>
$\approx h_0/4$		7.74E-08	7.73E-08	1.01E-10	4.35E-09	7.76E-08	<b>1.00</b>
$\approx h_0/8$		1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	<b>1.00</b>
$h_0$	<b>6</b>	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	<b>1.02</b>
$\approx h_0/2$		5.42E-08	5.42E-08	2.40E-10	4.02E-09	5.46E-08	<b>1.01</b>
$\approx h_0/4$		1.07E-09	1.07E-09	1.03E-11	6.90E-11	1.08E-09	<b>1.01</b>

# Uniform refinement: asymptotic exactness

$h$	$p$	$\ \nabla_d(u-u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	$\eta_{\text{osc}}$	$\ \nabla_d(u_h - S_h)\ $	$\eta$	$\eta^{\text{eff}}$
$h_0$	<b>1</b>	1.07E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	<b>1.17</b>
$\approx h_0/2$		5.56E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	<b>1.09</b>
$\approx h_0/4$		2.92E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	<b>1.06</b>
$\approx h_0/8$		1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	<b>1.04</b>
$h_0$	<b>2</b>	1.54E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	<b>1.06</b>
$\approx h_0/2$		4.07E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	<b>1.04</b>
$\approx h_0/4$		1.10E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	<b>1.03</b>
$\approx h_0/8$		2.50E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	<b>1.03</b>
$h_0$	<b>3</b>	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	<b>1.03</b>
$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	<b>1.01</b>
$\approx h_0/4$		2.60E-04	2.60E-04	4.73E-07	2.54E-05	2.62E-04	<b>1.01</b>
$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	<b>1.01</b>
$h_0$	<b>4</b>	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	<b>1.02</b>
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	<b>1.01</b>
$\approx h_0/4$		5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	<b>1.01</b>
$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	<b>1.01</b>
$h_0$	<b>5</b>	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	<b>1.02</b>
$\approx h_0/2$		2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	<b>1.01</b>
$\approx h_0/4$		7.74E-08	7.73E-08	1.01E-10	4.35E-09	7.76E-08	<b>1.00</b>
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$h_0$	<b>6</b>	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	<b>1.02</b>
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$h$	$p$	$\ \nabla_d(u-u_h)\ $	$\ \nabla_d u_h + \sigma_h\ $	$\eta_{\text{osc}}$	$\ \nabla_d(u_h - S_h)\ $	$\eta$	$\eta^{\text{eff}}$
$h_0$	<b>1</b>	1.07E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	<b>1.17</b>
$\approx h_0/2$		5.56E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	<b>1.09</b>
$\approx h_0/4$		2.92E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	<b>1.06</b>
$\approx h_0/8$		1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	<b>1.04</b>
$h_0$	<b>2</b>	1.54E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	<b>1.06</b>
$\approx h_0/2$		4.07E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	<b>1.04</b>
$\approx h_0/4$		1.10E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	<b>1.03</b>
$\approx h_0/8$		2.50E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	<b>1.03</b>
$h_0$	<b>3</b>	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	<b>1.03</b>
$\approx h_0/2$		1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	<b>1.01</b>
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$\approx h_0/8$		2.75E-05	2.75E-05	1.15E-08	2.55E-06	2.76E-05	<b>1.01</b>
$h_0$	<b>4</b>	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	<b>1.02</b>
$\approx h_0/2$		6.92E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	<b>1.01</b>
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$\approx h_0/8$		2.58E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	<b>1.01</b>
$h_0$	<b>5</b>	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	<b>1.02</b>
$\approx h_0/2$		2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	<b>1.01</b>
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$\approx h_0/8$		1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	<b>1.00</b>
$h_0$	<b>6</b>	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	<b>1.02</b>
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$h$	$p$	$\ \nabla_d(u-u_h)\ $	$\ u-u_h\ _{DG}$	$\ \nabla_d u_h + \sigma_h\ $	$\eta_{osc}$	$\ \nabla_d(u_h-s_h)\ $	$\eta$	$\eta_{DG}$	$J^{eff}$	$J_{DG}^{eff}$
$h_0$	<b>1</b>	1.07E-00	1.09E-00	1.12E-00	5.55E-02	4.16E-01	1.25E-00	1.26E-00	1.17	1.16
$\approx h_0/2$		5.56E-01	5.61E-01	5.71E-01	7.42E-03	1.82E-01	6.07E-01	6.11E-01	1.09	1.09
$\approx h_0/4$		2.92E-01	2.93E-01	2.96E-01	1.04E-03	8.77E-02	3.10E-01	3.11E-01	1.06	1.06
$\approx h_0/8$		1.39E-01	1.39E-01	1.40E-01	1.10E-04	3.85E-02	1.45E-01	1.45E-01	1.04	1.04
$h_0$	<b>2</b>	1.54E-01	1.55E-01	1.55E-01	5.10E-03	3.05E-02	1.63E-01	1.64E-01	1.06	1.06
$\approx h_0/2$		4.07E-02	4.09E-02	4.13E-02	3.53E-04	7.55E-03	4.23E-02	4.26E-02	1.04	1.04
$\approx h_0/4$		1.10E-02	1.11E-02	1.12E-02	2.51E-05	1.97E-03	1.14E-02	1.15E-02	1.03	1.03
$\approx h_0/8$		2.50E-03	2.52E-03	2.54E-03	1.30E-06	4.21E-04	2.57E-03	2.59E-03	1.03	1.03
$h_0$	<b>3</b>	1.37E-02	1.37E-02	1.37E-02	3.58E-04	1.74E-03	1.41E-02	1.41E-02	1.03	1.03
$\approx h_0/2$		1.85E-03	1.85E-03	1.85E-03	1.26E-05	2.10E-04	1.88E-03	1.88E-03	1.01	1.01
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$h_0$	<b>4</b>	9.87E-04	9.87E-04	9.84E-04	2.12E-05	1.11E-04	1.01E-03	1.01E-03	1.02	1.02
$\approx h_0/2$		6.92E-05	6.93E-05	6.92E-05	3.96E-07	7.44E-06	7.00E-05	7.00E-05	1.01	1.01
$\approx h_0/4$		5.04E-06	5.04E-06	5.04E-06	7.58E-09	4.98E-07	5.07E-06	5.07E-06	1.01	1.01
$\approx h_0/8$		2.58E-07	2.59E-07	2.58E-07	8.96E-11	2.47E-08	2.60E-07	2.60E-07	1.01	1.01
$h_0$	<b>5</b>	5.64E-05	5.64E-05	5.63E-05	1.06E-06	4.50E-06	5.75E-05	5.75E-05	1.02	1.02
$\approx h_0/2$		2.01E-06	2.01E-06	2.01E-06	9.88E-09	1.46E-07	2.03E-06	2.03E-06	1.01	1.01
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$\approx h_0/8$		1.86E-09	1.86E-09	1.86E-09	1.70E-12	1.00E-10	1.86E-09	1.86E-09	1.00	1.00
$h_0$	<b>6</b>	2.85E-06	2.85E-06	2.85E-06	4.70E-08	2.18E-07	2.90E-06	2.90E-06	1.02	1.02
$\approx h_0/2$		5.42E-08	5.42E-08	5.42E-08	2.40E-10	4.02E-09	5.46E-08	5.46E-08	1.01	1.01
$\approx h_0/4$		1.07E-09	1.07E-09	1.07E-09	1.03E-11	6.90E-11	1.08E-09	1.08E-09	1.01	1.01

# Numerics: singular case

## Model problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega &:= (-1, 1)^2 \setminus [0, 1]^2, \\ u &= u_D & \text{on } \partial\Omega \end{aligned}$$

## Exact solution

$$u(r, \phi) = r^{2/3} \sin(2\phi/3)$$

## Discretization

- incomplete interior penalty discontinuous Galerkin method
- unstructured non-nested triangular grids
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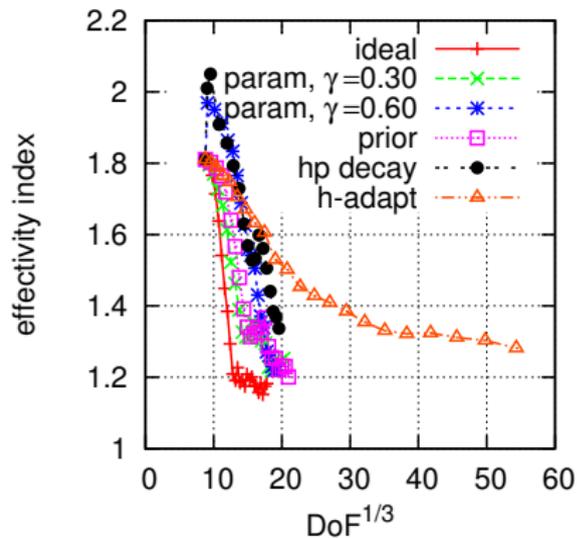
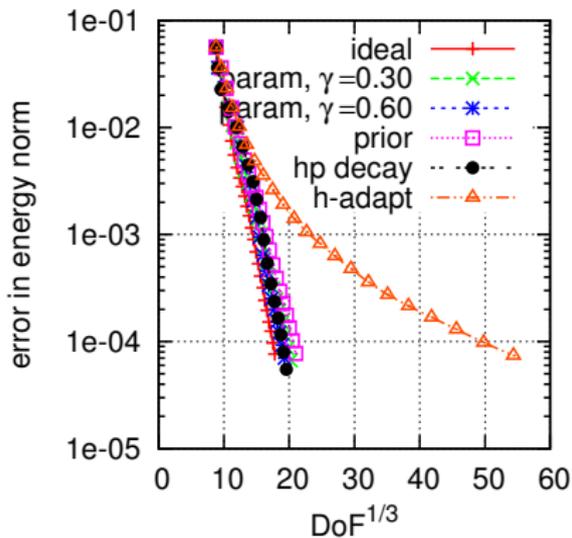
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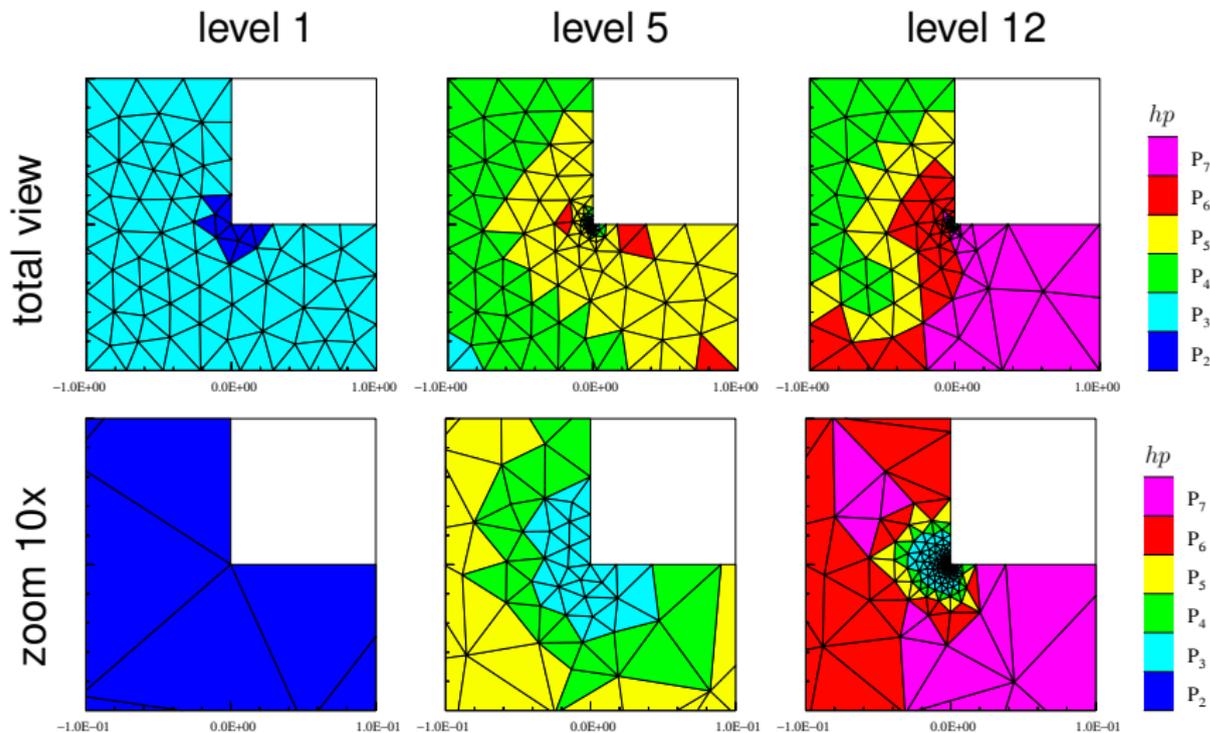
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# hp-adaptive refinement: exponential convergence



# hp-refinement grids



# Outline

- 1 Introduction
- 2 Laplace equation: potential & flux reconstructions
  - Guaranteed upper bound in a unified framework
  - Polynomial-degree-robust local efficiency
  - Applications & numerical results
- 3 Nonlinear Laplace equation: adaptive stopping criteria**
  - Adaptive inexact Newton method
  - Applications & numerical results
- 4 Laplace eigenvalues and eigenvectors: guaranteed bounds
  - Applications & numerical results
- 5 Heat equation: robustness wrt final time & local efficiency
- 6 Two-phase flow in porous media: industrial application
- 7 Conclusions and outlook

# 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.
 
$$\mathbb{A}^{k-1} U^k \approx F^{k-1}.$$
- 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.)
 
$$\mathbb{A}^{k-1} U^{k,i} = F^{k-1} - R^{k,i}.$$
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  - 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.
  - 4 Convergence? OK  $\Rightarrow$  finish. KO  $\Rightarrow k := k + 1$ , back to 2.

# 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.
 
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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 Eisenstat and Walker (1990's), Becker, Johnson, and Rannacher (1995), Deuffhard (2004 book), Arioli (2000's))

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

Question (Error Verfürth (1994), Carstensen and Klose (2003), Chaillou and Suri (2006), Kim (2007))

- *How big is the error  $\|u - u_h^{k,i}\|_{?,\Omega}$  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

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

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

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

## 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

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

## Intrinsic error measure

$$\mathcal{J}_u(u_h^{k,i}) := \underbrace{\sup_{\varphi \in V; \|\nabla\varphi\|_p=1} (\bar{\sigma}(u, \nabla u) - \bar{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}), \nabla\varphi)}_{\text{dual norm of the residual}} + \underbrace{\left\{ \sum_{K \in \mathcal{T}_h} \sum_{\theta \in \mathcal{E}_K} h_e^{1-q} \|\llbracket u - u_h^{k,i} \rrbracket\|_{q,e}^q \right\}^{1/q}}_{\text{distance of } u_h \text{ to } V}$$

✓ 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  $\sigma_h^{k,i} \in \mathbf{H}^q(\text{div}, \Omega)$  such that

$$\nabla \cdot \sigma_h^{k,i} = f.$$

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

There exist fluxes  $\sigma_{h,\text{dis}}^{k,i}, \sigma_{h,\text{lin}}^{k,i}, \sigma_{h,\text{alg}}^{k,i} \in [L^q(\Omega)]^d$  such that

- (i)  $\sigma_h^{k,i} = \sigma_{h,\text{dis}}^{k,i} + \sigma_{h,\text{lin}}^{k,i} + \sigma_{h,\text{alg}}^{k,i}$ ;
- (ii) as the linear solver converges,  $\|\sigma_{h,\text{alg}}^{k,i}\|_q \rightarrow 0$ ;
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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 (up to quadrature and data oscillation)

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

# Estimators

- *discretization* estimator

$$\eta_{\text{disc},K}^{k,i} := 2^{\frac{1}{p}} \left( \|\bar{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}) + \sigma_{h,\text{dis}}^{k,i}\|_{q,K} + \left\{ \sum_{e \in \mathcal{E}_K} h_e^{1-q} \|[u_h^{k,i}]\|_{q,e}^q \right\}^{1/q} \right)$$

- *linearization* estimator

$$\eta_{\text{lin},K}^{k,i} := \|\sigma_{h,\text{lin}}^{k,i}\|_{q,K}$$

- *algebraic* estimator

$$\eta_{\text{alg},K}^{k,i} := \|\sigma_{h,\text{alg}}^{k,i}\|_{q,K}$$

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

# Stopping criteria: error components of similar size

## Global stopping criteria

- stop whenever:

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

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

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

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## Comments

- ✓ same physical units (fluxes)
- ✓ naturally relative
- ✓ proper  $[L^q(\Omega)]^d$  framework  $\times$   $l_2$  norms of algebraic vectors

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# Global efficiency

## Theorem (Global efficiency)

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

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

where *C* is independent of  $\bar{\sigma}$  and *q*.

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## Discretization methods

- ✓ conforming finite elements
- ✓ nonconforming finite elements
- ✓ discontinuous Galerkin
- ✓ various finite volumes
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- ✓ fixed point
- ✓ Newton

## Linear solvers

- ✓ independent of the linear solver

... all Assumptions A to D verified



informatics mathematics  
*Inria*



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# Numerical experiment I

## Model problem

- $p$ -Laplacian

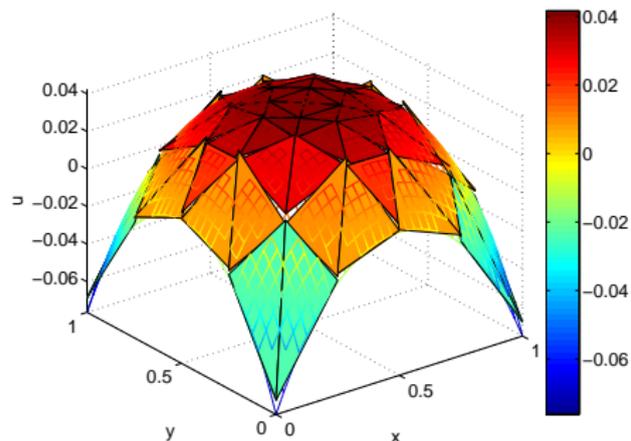
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_D && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

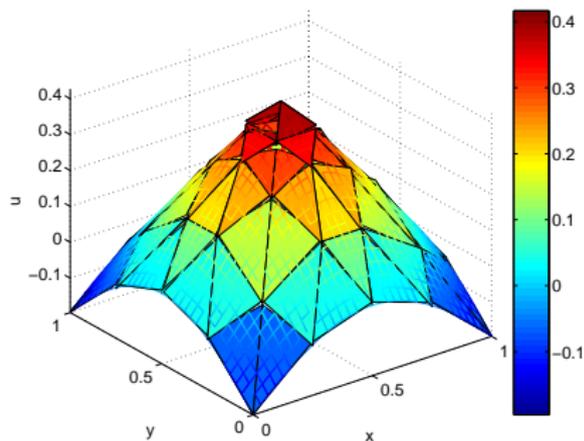
$$u(x, y) = -\frac{p-1}{p} \left( \left(x - \frac{1}{2}\right)^2 + \left(y - \frac{1}{2}\right)^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

# Analytical and approximate solutions

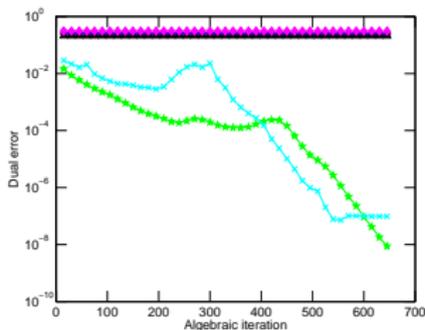


Case  $p = 1.5$

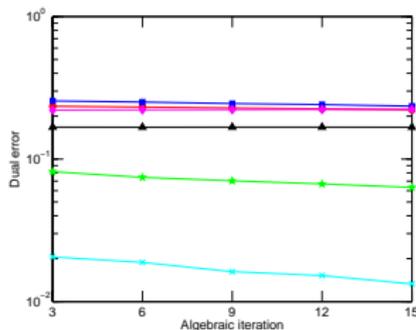


Case  $p = 10$

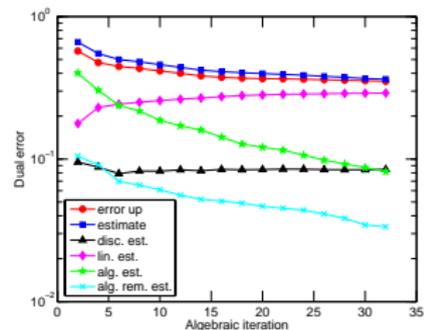
# Error and estimators as a function of CG iterations, $\rho = 10$ , 6th level mesh, 6th Newton step



Newton

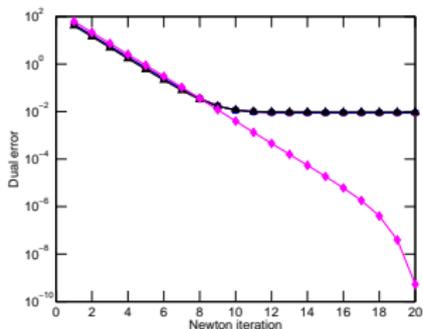


inexact Newton

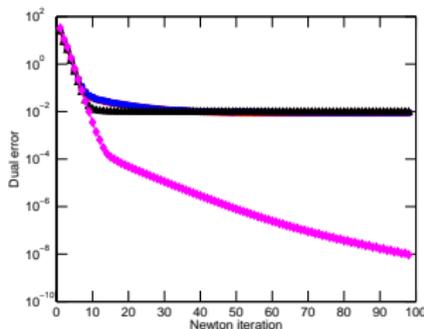


ad. inexact Newton

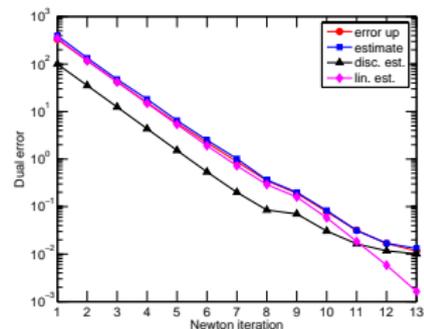
# Error and estimators as a function of Newton iterations, $p = 10$ , 6th level mesh



Newton

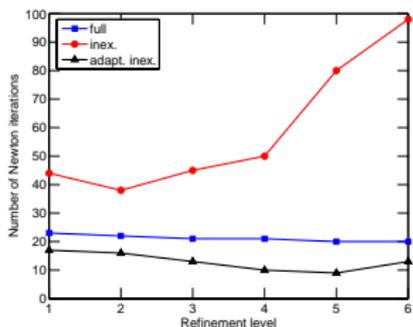


inexact Newton

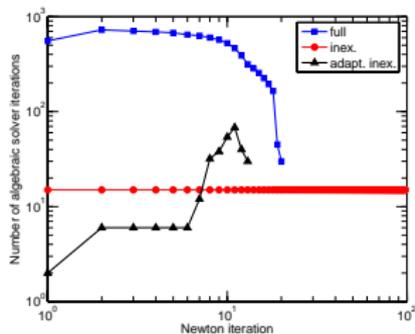


ad. inexact Newton

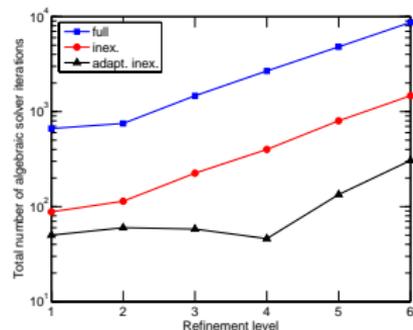
# Newton and algebraic iterations, $p = 10$



Newton it. / refinement

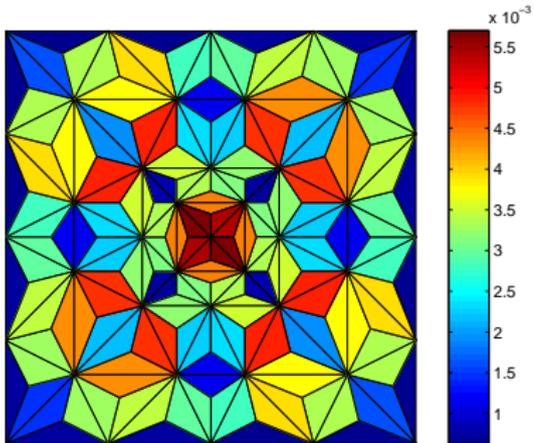


alg. it. / Newton step

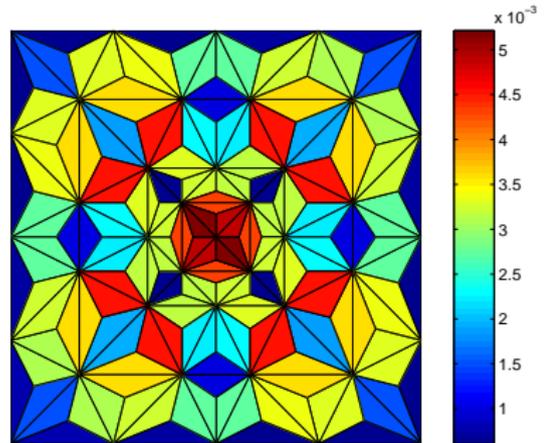


alg. it. / refinement

# Error distribution, $p = 10$

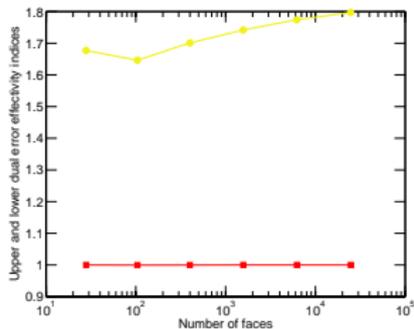


Estimated error distribution

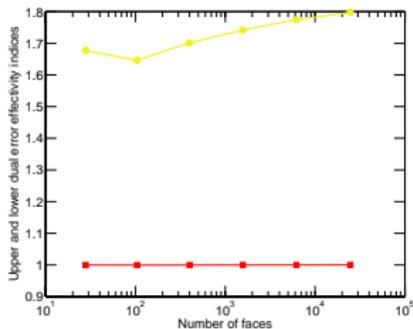


Exact error distribution

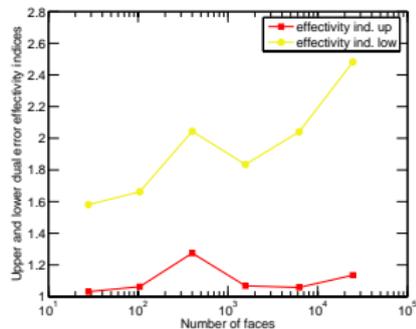
# Effectivity indices, $p = 10$



Newton

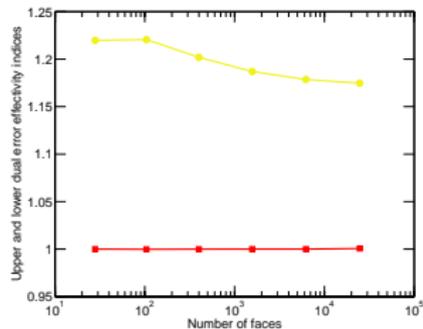


inexact Newton

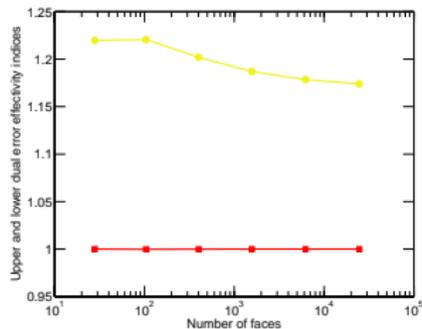


ad. inexact Newton

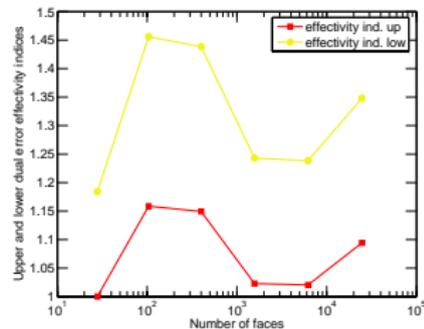
# Effectivity indices, $p = 1.5$



Newton



inexact Newton



ad. inexact Newton

# Numerical experiment II

## Model problem

- $p$ -Laplacian

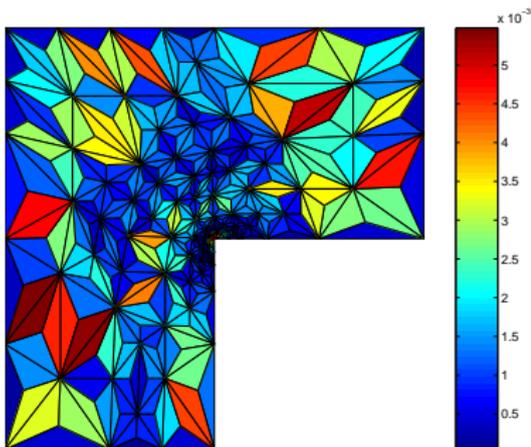
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_D && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

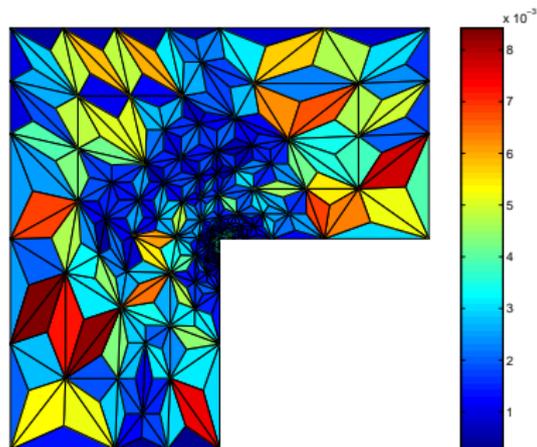
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

# Error distribution on an adaptively refined mesh

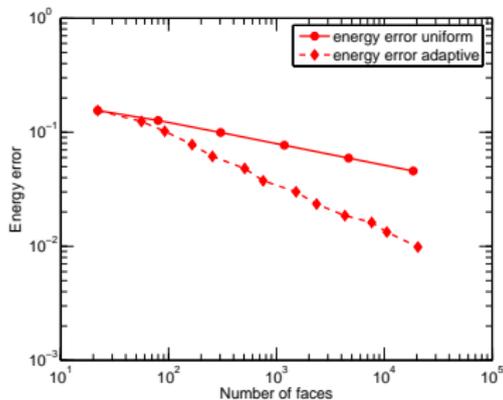


Estimated error distribution

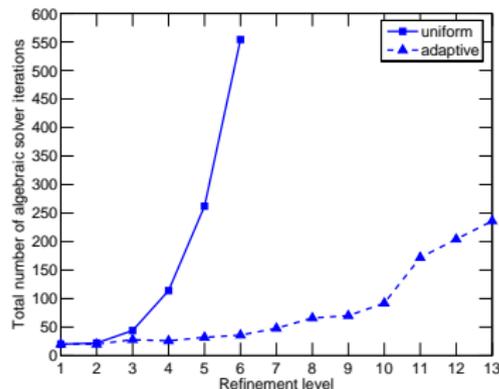


Exact error distribution

# Energy error and overall performance



Energy error



Overall performance

# Outline

- 1 Introduction
- 2 Laplace equation: potential & flux reconstructions
  - Guaranteed upper bound in a unified framework
  - Polynomial-degree-robust local efficiency
  - Applications & numerical results
- 3 Nonlinear Laplace equation: adaptive stopping criteria
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- 7 Conclusions and outlook

# Laplace eigenvalue problem

## Problem

Find **eigenvector & eigenvalue pair**  $(u, \lambda)$  such that

$$\begin{aligned} -\Delta u &= \lambda u && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$

## Weak formulation

Find  $(u_i, \lambda_i) \in V \times \mathbb{R}^+$ ,  $i \geq 1$ , with  $\|u_i\| = 1$ , such that

$$(\nabla u_i, \nabla v) = \lambda_i (u_i, v) \quad \forall v \in V.$$

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# Main results (conforming setting)

## Assumption A (Conforming variational solution)

There holds

- $(u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+$
- $\|u_{ih}\| = 1$
- $\|\nabla u_{ih}\|^2 = \lambda_{ih} \quad (\Rightarrow \lambda_{1h} \geq \lambda_1)$

We bound

- $i$ -th eigenvector energy error

$$\|\nabla(u_i - u_{ih})\| \leq \sqrt{\lambda_i - \lambda_{ih}}$$

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## We bound

- 1  $i$ -th eigenvalue error

$$\lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2$$

- 2  $i$ -th eigenvector energy error

$$\|\nabla(u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih})$$

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$$\|\nabla(u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \leq C_{\text{eff},i} \|\nabla(u_i - u_{ih})\|$$

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## We bound

- 1  $i$ -th eigenvalue error

$$\lambda_{ih} - \lambda_i \leq \eta_i(u_{ih}, \lambda_{ih})^2$$

- 2  $i$ -th eigenvector energy error

$$\|\nabla(u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih}) \leq C_{\text{eff},i} \|\nabla(u_i - u_{ih})\|$$

- ✓  $C_{\text{eff},i}$  only depends on mesh shape regularity and on

$$\max \left\{ \left( \frac{\lambda_i}{\lambda_{i-1}} - 1 \right)^{-1}, \left( 1 - \frac{\lambda_i}{\lambda_{i+1}} \right)^{-1} \right\} \frac{\lambda_i}{\lambda_1}$$

- ✓ we give computable upper bounds on  $C_{\text{eff},i}$

# Main results (conforming setting)

## Assumption A (Conforming variational solution)

There holds

- $(u_{ih}, \lambda_{ih}) \in V \times \mathbb{R}^+$
- $\|u_{ih}\| = 1$
- $\|\nabla u_{ih}\|^2 = \lambda_{ih} \quad (\Rightarrow \lambda_{1h} \geq \lambda_1)$

## We bound

$i$ -th eigenvalue upper and lower bounds

$$\lambda_{ih} - \eta_i(u_{ih}, \lambda_{ih})^2 \leq \lambda_i \leq \lambda_{ih} - \tilde{\eta}_i(u_{ih}, \lambda_{ih})^2$$

②  $i$ -th eigenvector energy error

$$\|\nabla(u_i - u_{ih})\| \leq \eta_i(u_{ih}, \lambda_{ih})$$

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# Unit square

## Setting

- $\Omega = (0, 1)^2$
- $\lambda_1 = 2\pi^2$ ,  $\lambda_2 = 5\pi^2$  known explicitly
- $u_1(x, y) = \sin(\pi x) \sin(\pi y)$  known explicitly

## Effectivity indices

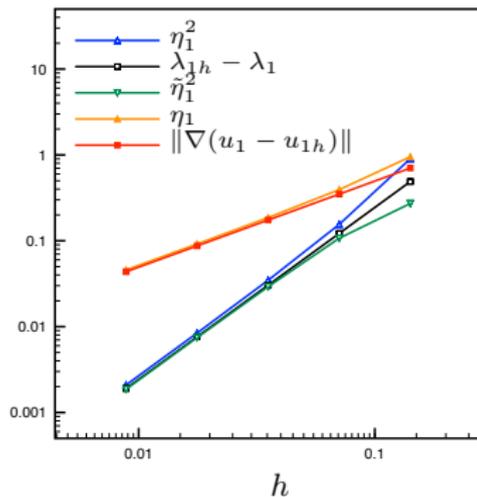
- recall  $\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2$

$$I_{\lambda, \text{eff}}^{\text{lb}} := \frac{\lambda_{ih} - \lambda_i}{\tilde{\eta}_i^2}, \quad I_{\lambda, \text{eff}}^{\text{ub}} := \frac{\eta_i^2}{\lambda_{ih} - \lambda_i}$$

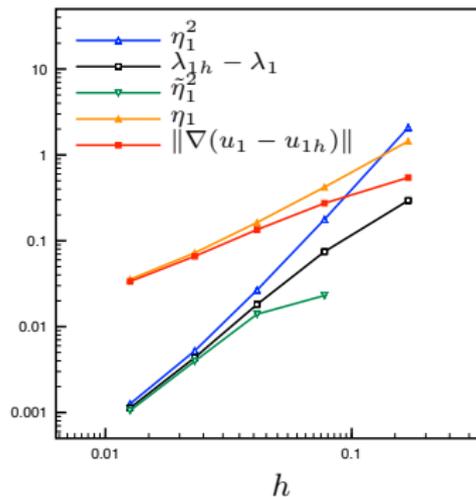
- recall  $\|\nabla(u_i - u_{ih})\| \leq \eta_i$

$$I_{u, \text{eff}}^{\text{ub}} := \frac{\eta_i}{\|\nabla(u_i - u_{ih})\|}$$

# Conforming finite elements



Structured meshes



Unstructured meshes

# Conforming finite elements

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
10	0.1414	121	19.7392	20.2284	19.5054	19.8667	1.35	1.48	1.84E-02	1.21
20	0.0707	441	19.7392	19.8611	19.7164	19.7486	1.08	1.19	1.63E-03	1.09
40	0.0354	1,681	19.7392	19.7696	19.7356	19.7401	1.03	1.12	2.28E-04	1.06
80	0.0177	6,561	19.7392	19.7468	19.7384	19.7393	1.02	1.10	4.56E-05	1.05
160	0.0088	25,921	19.7392	19.7411	19.7390	19.7392	1.02	1.10	1.01E-05	1.05

## Structured meshes

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
10	0.1698	143	19.7392	20.0336	18.8265	—	—	4.10	—	2.02
20	0.0776	523	19.7392	19.8139	19.6820	19.7682	1.63	1.77	4.37E-03	1.33
40	0.0413	1,975	19.7392	19.7573	19.7342	19.7416	1.15	1.28	3.75E-04	1.13
80	0.0230	7,704	19.7392	19.7436	19.7386	19.7395	1.07	1.14	4.56E-05	1.07
160	0.0126	30,666	19.7392	19.7403	19.7391	19.7393	1.06	1.10	1.01E-05	1.05

## Unstructured meshes

# Conforming finite elements

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
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## Unstructured meshes

# Conforming finite elements

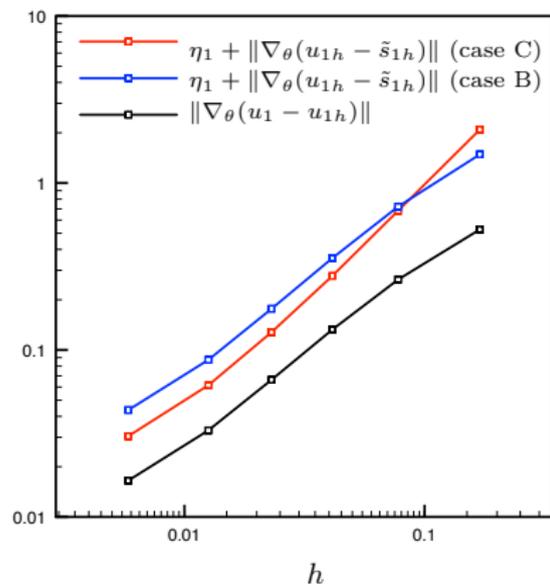
$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
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## Structured meshes

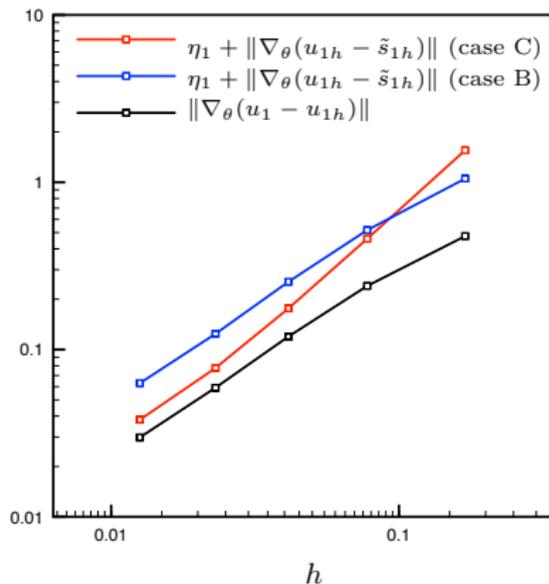
$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\lambda_{1h} - \eta_1^2$	$\lambda_{1h} - \tilde{\eta}_1^2$	$I_{\lambda,\text{eff}}^{\text{lb}}$	$I_{\lambda,\text{eff}}^{\text{ub}}$	$E_{\lambda,\text{rel}}$	$I_{u,\text{eff}}^{\text{ub}}$
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## Unstructured meshes

# Nonconforming finite elements & DG's



Nonconforming finite elements



Discontinuous Galerkin

# Nonconforming finite elements & DG's

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\ell_{u,eff}^{ub}$
10	0.1414	320	19.7392	19.6850	18.8966	19.8262	4.80e-02	2.68
20	0.0707	1240	19.7392	19.7257	19.6495	19.7616	5.69e-03	2.11
40	0.0354	4880	19.7392	19.7358	19.7246	19.7448	1.02e-03	1.91
80	0.0177	19360	19.7392	19.7384	19.7361	19.7406	2.29e-04	1.85
160	0.0088	77120	19.7392	19.7390	19.7385	19.7396	5.53e-05	1.83
320	0.0044	307840	19.7392	19.7392	19.7390	19.7393	1.37e-05	1.83

## Nonconforming finite elements

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\ell_{u,eff}^{ub}$
10	0.1698	732	19.7392	19.9432	17.8788	19.9501	1.10e-01	3.26
20	0.0776	2892	19.7392	19.7928	19.6264	19.7939	8.50e-03	1.91
40	0.0413	11364	19.7392	19.7526	19.7295	19.7529	1.18e-03	1.47
80	0.0230	45258	19.7392	19.7425	19.7381	19.7426	2.28e-04	1.31
160	0.0126	182070	19.7392	19.7400	19.7390	19.7401	5.35e-05	1.28

## SIP discontinuous Galerkin

# Nonconforming finite elements & DG's

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\Gamma_{u,eff}^{ub}$
10	0.1414	320	19.7392	19.6850	18.8966	19.8262	4.80e-02	2.68
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160	0.0088	77120	19.7392	19.7390	19.7385	19.7396	5.53e-05	1.83
320	0.0044	307840	19.7392	19.7392	19.7390	19.7393	1.37e-05	1.83

## Nonconforming finite elements

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\Gamma_{u,eff}^{ub}$
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40	0.0413	11364	19.7392	19.7526	19.7295	19.7529	1.18e-03	1.47
80	0.0230	45258	19.7392	19.7425	19.7381	19.7426	2.28e-04	1.31
160	0.0126	182070	19.7392	19.7400	19.7390	19.7401	5.35e-05	1.28

## SIP discontinuous Galerkin

# Nonconforming finite elements & DG's

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\Gamma_{U,eff}^{ub}$
10	0.1414	320	19.7392	19.6850	18.8966	19.8262	4.80e-02	2.68
20	0.0707	1240	19.7392	19.7257	19.6495	19.7616	5.69e-03	2.11
40	0.0354	4880	19.7392	19.7358	19.7246	19.7448	1.02e-03	1.91
80	0.0177	19360	19.7392	19.7384	19.7361	19.7406	2.29e-04	1.85
160	0.0088	77120	19.7392	19.7390	19.7385	19.7396	5.53e-05	1.83
320	0.0044	307840	19.7392	19.7392	19.7390	19.7393	1.37e-05	1.83

## Nonconforming finite elements

$N$	$h$	ndof	$\lambda_1$	$\lambda_{1h}$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2} - \eta_1^2$	$\frac{\ \nabla s_{1h}\ ^2}{\ s_{1h}\ ^2}$	$E_{\lambda,rel}$	$\Gamma_{U,eff}^{ub}$
10	0.1698	732	19.7392	19.9432	17.8788	19.9501	1.10e-01	3.26
20	0.0776	2892	19.7392	19.7928	19.6264	19.7939	8.50e-03	1.91
40	0.0413	11364	19.7392	19.7526	19.7295	19.7529	1.18e-03	1.47
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# Model parabolic problem

## The heat equation

$$\begin{aligned} \partial_t u - \Delta u &= f && \text{in } \Omega \times (0, T), \\ u &= 0 && \text{on } \partial\Omega \times (0, T), \\ u(0) &= u_0 && \text{in } \Omega \end{aligned}$$

## Spaces

$$X := L^2(0, T; H_0^1(\Omega)),$$

$$\|v\|_X^2 := \int_0^T \|\nabla v\|^2 dt,$$

$$Y := L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; H^{-1}(\Omega)),$$

$$\|v\|_Y^2 := \int_0^T \|\partial_t v\|_{H^{-1}(\Omega)}^2 + \|\nabla v\|^2 dt + \|v(T)\|^2$$

## Weak solution

Find  $u \in Y$  with  $u(0) = u_0$  such that

$$\int_0^T \langle \partial_t u, v \rangle + (\nabla u, \nabla v) dt = \int_0^T (f, v) dt \quad \forall v \in X.$$

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# Error and residual in the unsteady case

## Theorem (Parabolic inf-sup identity)

For every  $\varphi \in Y$ , we have

$$\|\varphi\|_Y^2 = \left[ \sup_{v \in X, \|v\|_X=1} \int_0^T \langle \partial_t \varphi, v \rangle + (\nabla \varphi, \nabla v) dt \right]^2 + \|\varphi(0)\|^2.$$

## Residual of $u_{h\tau} \in Y$

- $\mathcal{R}(u_{h\tau}) \in X'$ , the misfit of  $u_{h\tau}$  in the weak formulation:

$$\langle \mathcal{R}(u_{h\tau}), v \rangle := \int_0^T (f, v) - \langle \partial_t u_{h\tau}, v \rangle - (\nabla u_{h\tau}, \nabla v) dt$$

- dual norm of the residual

$$\|\mathcal{R}(u_{h\tau})\|_{X'} := \sup_{v \in X, \|v\|_X=1} \langle \mathcal{R}(u_{h\tau}), v \rangle$$

$Y$  norm error is the dual  $X$  norm of the residual + IC error

$$\|u - u_{h\tau}\|_Y^2 = \|\mathcal{R}(u_{h\tau})\|_{X'}^2 + \|u_0 - u_{h\tau}(0)\|^2$$

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# A posteriori estimate

## Guaranteed upper bound

- ✓  $\|u - u_{h\tau}\|_{\mathcal{E}_{Y,\Omega \times (0,T)}}^2 \leq \sum_{n=1}^N \sum_{K \in \mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2$
- ✓ no undetermined constant: **error control**

## Local space-time efficiency

- ✓  $\eta_K^n(u_{h\tau}) \leq C_{\text{eff}} \|u - u_{h\tau}\|_{\mathcal{E}_{Y,\text{neighbors of } K \times (t^{n-1}, t^n)}}$
- ✓ optimal space-time mesh refinement
- ✓ **local** in **time** and in **space** error lower bound

## Robustness

- ✓  $C_{\text{eff}}$  independent of data, domain  $\Omega$ , **final time**  $T$ , meshes, solution  $u$ , **polynomial degrees** of  $u_{h\tau}$  in space and in time

## Asymptotic exactness

- ✓  $\sum_{n=1}^N \sum_{K \in \mathcal{T}_h^n} \eta_K^n(u_{h\tau})^2 / \|u - u_{h\tau}\|_{\mathcal{E}_{Y,\Omega \times (0,T)}}^2 \searrow 1$
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## Small evaluation cost

- ✓ estimators can be evaluated cheaply (locally)

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# Multiphase, multi-compositional flows

## Two-phase immiscible incompressible flow

$$\begin{aligned} \partial_t(\phi \mathbf{s}_\alpha) + \nabla \cdot \mathbf{u}_\alpha &= q_\alpha, & \alpha \in \{o, w\}, \\ -\lambda_\alpha(\mathbf{s}_w) \underline{\mathbf{K}}(\nabla p_\alpha + \rho_\alpha \mathbf{g} \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{o, w\}, \\ \mathbf{s}_o + \mathbf{s}_w &= \mathbf{1}, \\ p_o - p_w &= p_c(\mathbf{s}_w) \end{aligned}$$

+ boundary & initial conditions

### Mathematical issues

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

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

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

### Error components

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

### Full adaptivity

- only a **necessary number** of all **solver iterations**
- **“online decisions”**:  
algebraic step / linearization step / space mesh refinement / time step modification

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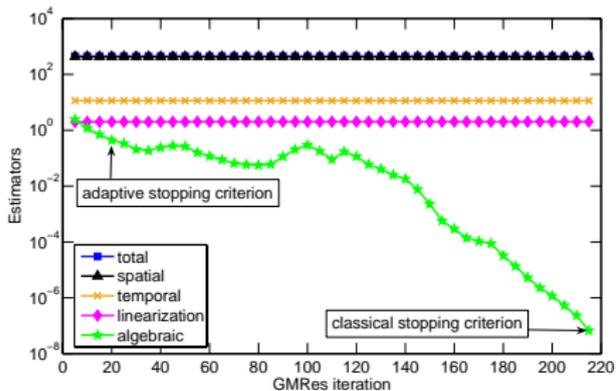
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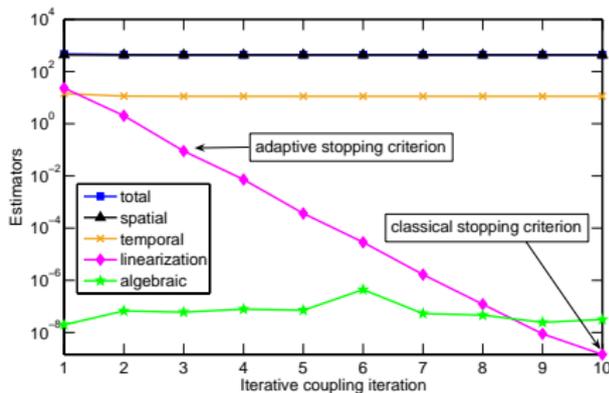
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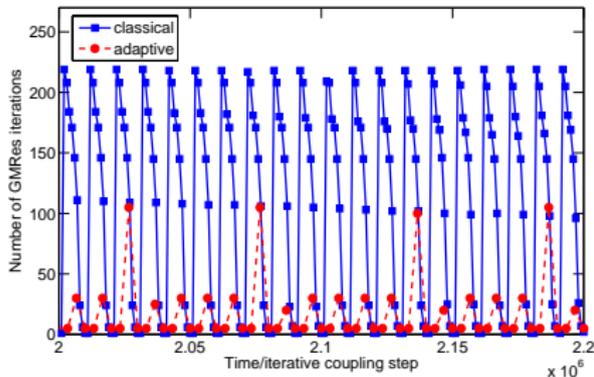


Estimators in function of GMRes iterations

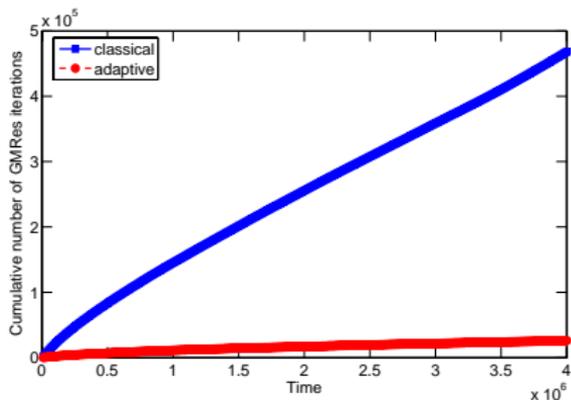


Estimators in function of iterative coupling iterations

# GMRes iterations

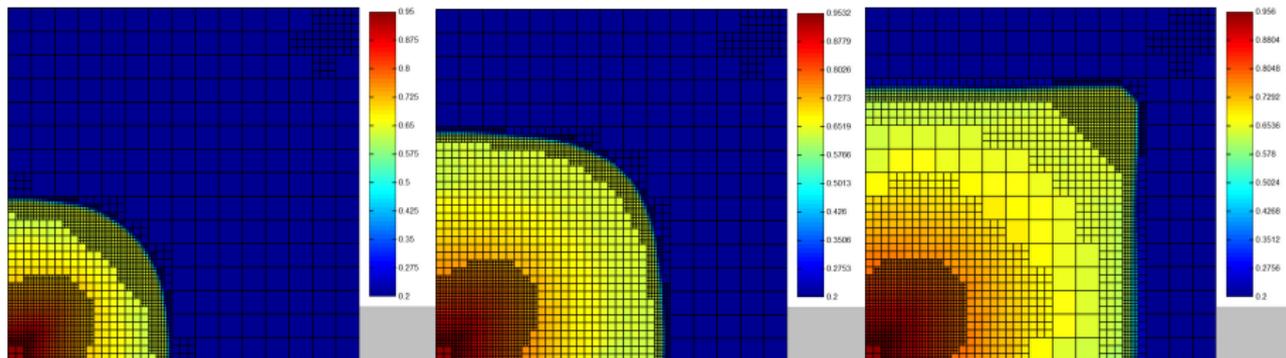


Per time and iterative coupling step



Cumulated

# Space/time/nonlinear solver/linear solver adaptivity



Fully adaptive computation

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- ✓ robustness (polynomial degree, final time)
- ✓ local (space-time) efficiency
- ✓ unified framework for all classical numerical schemes
- ✓ cover the set of basic model problems (also variational inequalities, Stokes, changing coefficients,  $H^{-1}$  source terms. . .)

## Ongoing work

- guaranteed reduction factor for  $hp$  refinement strategies
- convergence and optimality

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Thank you for your attention!

