A posteriori error estimates & adaptivity with balancing of error components

Martin Vohralík

Inria Paris & Ecole des Ponts

Paris, October 8, 2019

Outline

Numerical approximations of PDEs

Numerical methods

- mathematically-based algorithms evaluated by **computers**
- deliver **approximate solutions**
- conception: more effort $\Rightarrow$ closer to the unknown solution
- example: elastic rod

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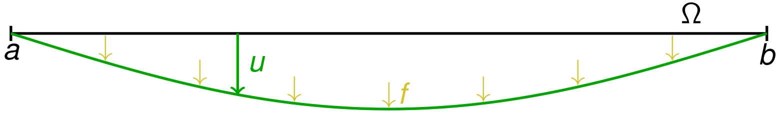

Numerical approximation u_h and its convergence to u

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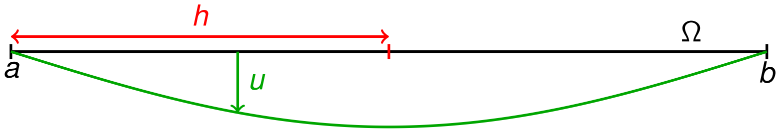

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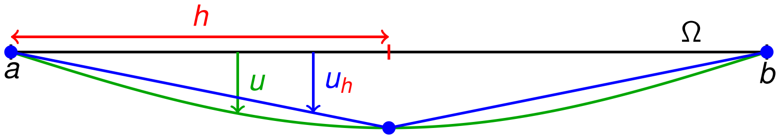

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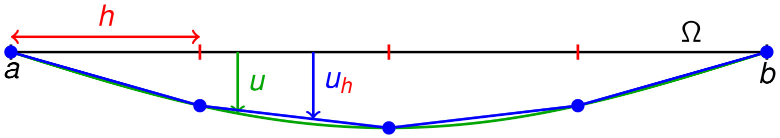

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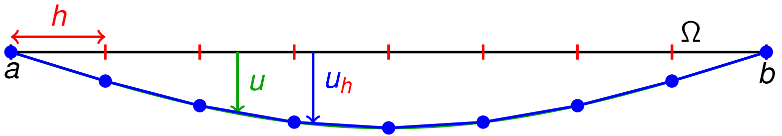

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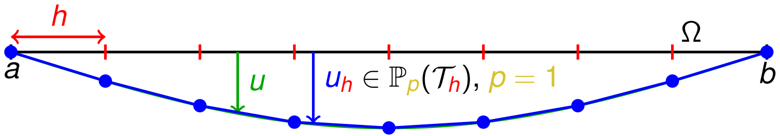

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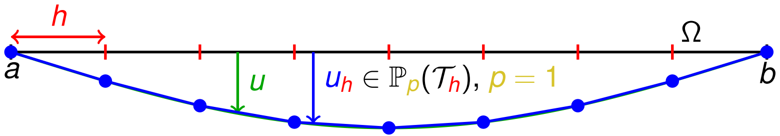

Numerical approximation u_h and its convergence to u

Error

$$\|\nabla(u - u_h)\| = \left\{\int_a^b |(u - u_h)'|^2\right\}^{\frac{1}{2}}$$

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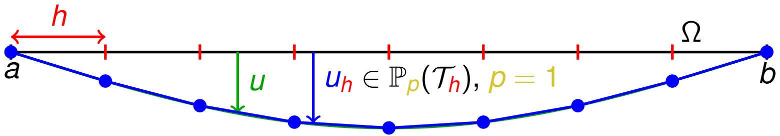

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$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

Need to solve

$$\mathbb{A}_h \mathrm{U}_h = \mathrm{F}_h$$

3 crucial questions

Crucial questions

1. How **large** is the overall **error**?
2. **Where** (model/space/time/lineariza-tion/algebra) is it **localized**?
3. Can we **decrease** it **efficiently**?

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1. **A posteriori** error **estimates**.

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Assumptions

- We know the data.
- The computer implementation and execution of our certification methodology is safe and correct.

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- deterministic, steady problem, PDE known, data known, implementation OK

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I believe **without error certification**

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CrossMark

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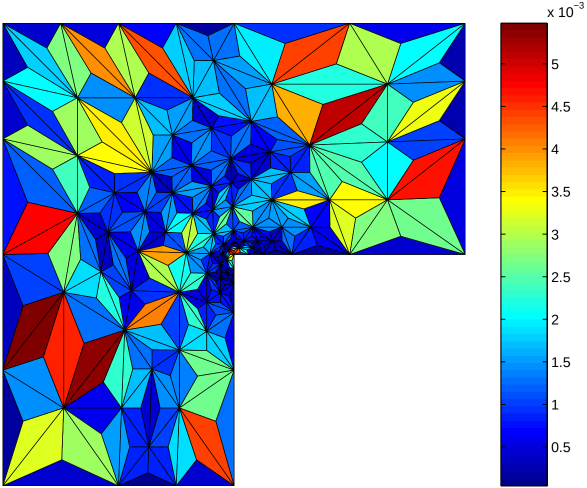
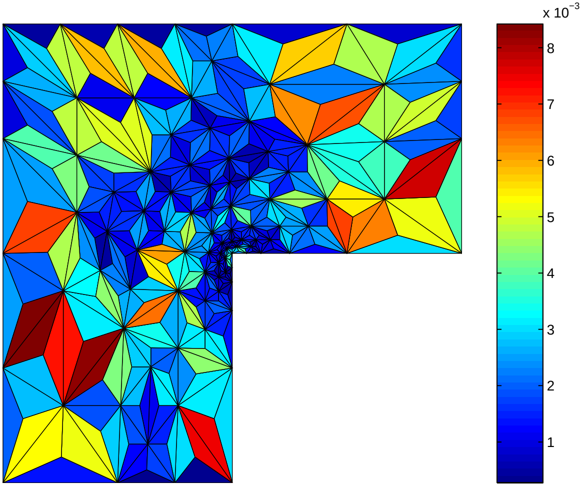
Appetizer: **it works!** (nonlinear problem with linearization & algebra)



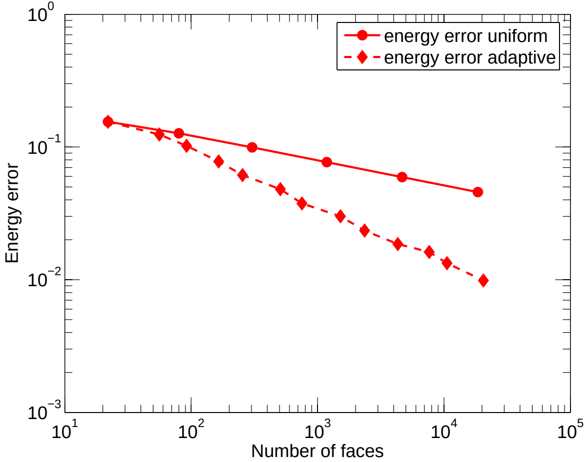
Estimated error distribution



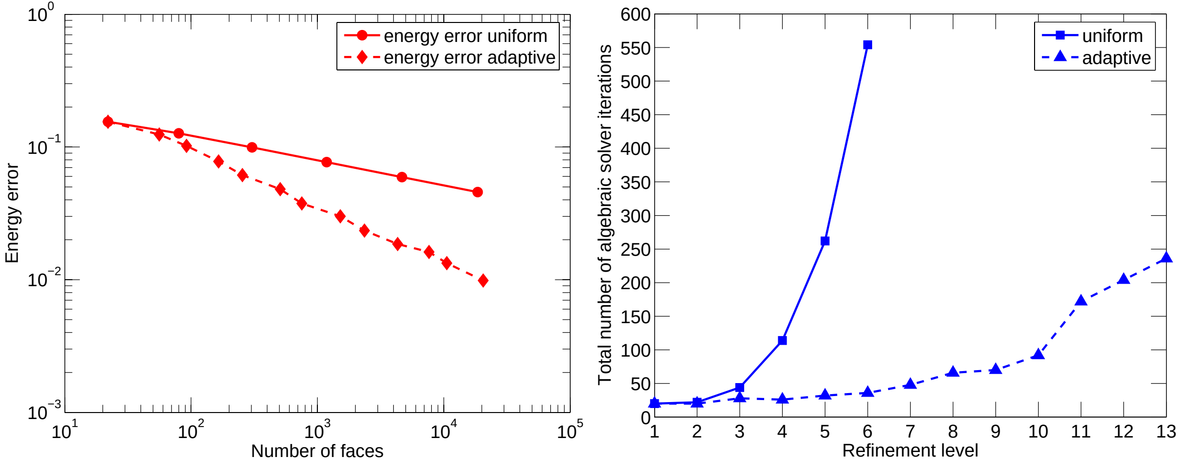
Exact error distribution

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Commercial: get more



Commercial: get more, pay less! (balancing all error components)



A posteriori error estimates: control the error

Elastic membrane equation

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

Guaranteed error upper bound (reliability)

$$\underbrace{\|\nabla(u - u_h)\|}_{\text{unknown error}} \le \underbrace{\eta(u_h)}_{\text{computable estimator}}$$

Error lower bound (efficiency)

$$\eta(u_h) \le C_{\text{eff}} \|\nabla(u - u_h)\|$$

- C_{eff} independent of Ω, u, u_h, h, p
- computable bound on C_{eff} available, $C_{\text{eff}} \approx 5$
- Prager and Synge (1947), Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Braess, Pillwein, & Schöberl (2009), Ern & Vohralík (2015)

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How large is the overall error? (model pb, known sol.)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\lVert\nabla u_h\rVert}$	$\lVert\nabla(u - u_h)\rVert$	rel. error $\frac{\lVert\nabla(u-u_h)\rVert}{\lVert\nabla u_h\rVert}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\lVert\nabla(u-u_h)\rVert}$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		$6.07 \times 10^{[illegible]}$				
$\approx h_0/4$		$3.10 \times 10^{[illegible]}$				
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A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)

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V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

How large is the overall error? (model pb, known sol.)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\text{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.25	28%	1.07	24%	**1.17**
$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}	13%	**1.09**
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}	6.6%	**1.06**
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}	3.1%	**1.04**
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}	9.2×10^{-1}%	**1.04**
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3}%	2.60×10^{-4}	5.9×10^{-3}%	**1.01**
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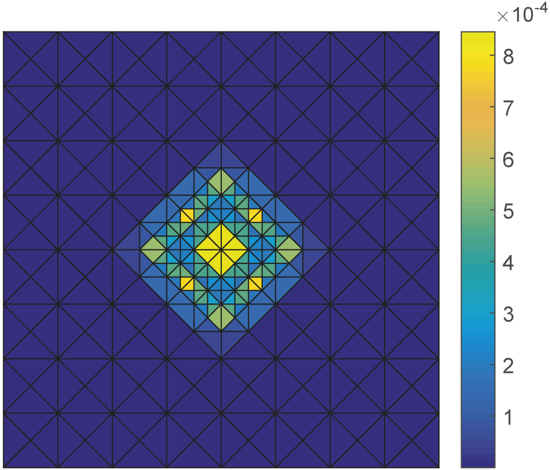
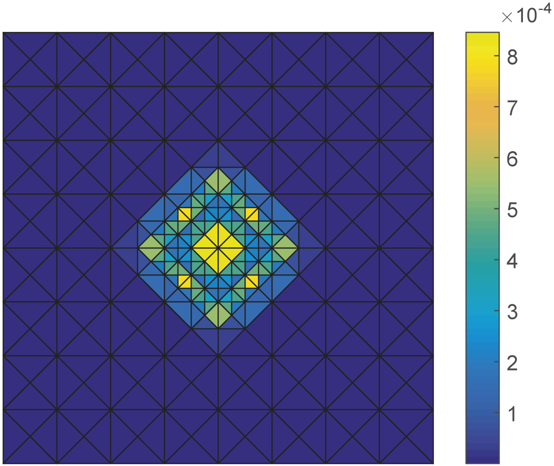
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

Where (in space) is the error localized?



Estimated error distribution $\eta_K(u_h)$



Exact error distribution $\|\nabla(u - u_h)\|_K$

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Adaptive mesh refinement (linear problem with exact solvers)

Adaptive mesh refinement

- Dörfler marking: subset $\mathcal{M}_\ell$ containing θ-fraction of the estimates

$$\sum_{K\in\mathcal{M}_\ell} \eta_K(u_\ell)^2 \geq \theta^2 \sum_{K\in\mathcal{T}_\ell} \eta_K(u_\ell)^2$$

Convergence on a sequence of adaptively refined meshes

- $$\|\nabla(u-u_\ell)\| \to 0$$
- some mesh elements may not be refined at all: ~~$h \searrow 0$~~
- Babuška & Miller (1987), Dörfler (1996)

Optimal error decay rate wrt degrees of freedom

- $$\|\nabla(u-u_\ell)\| \lesssim |\mathrm{DoF}_\ell|^{-p/d} \quad \text{(replaces } h^p\text{)}$$
- same for smooth & singular solutions: ~~higher-order only pay-off for sm. sol.~~
- decays to zero as fast as on a best-possible sequence of meshes
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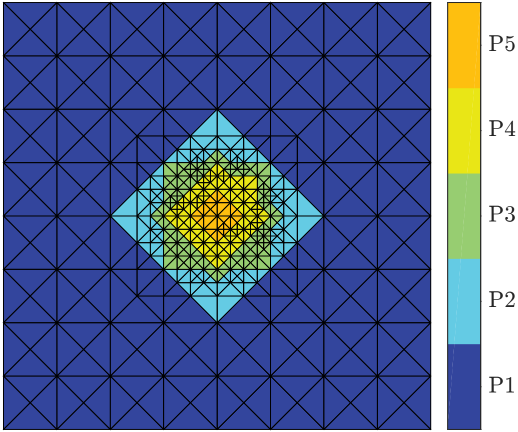

Mesh $\mathcal{T}_\ell$ and pol. degrees p_K

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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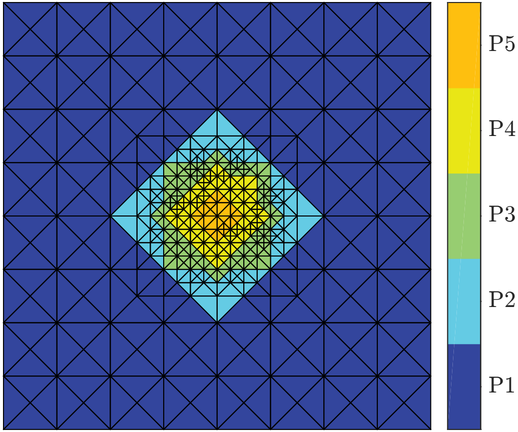

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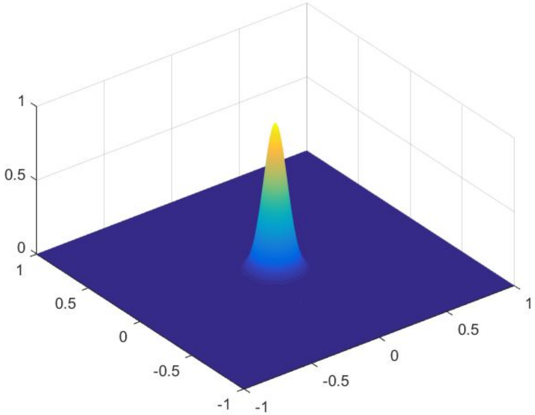

Exact solution

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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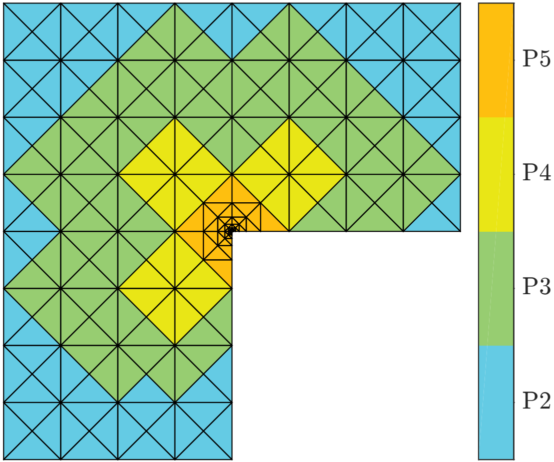

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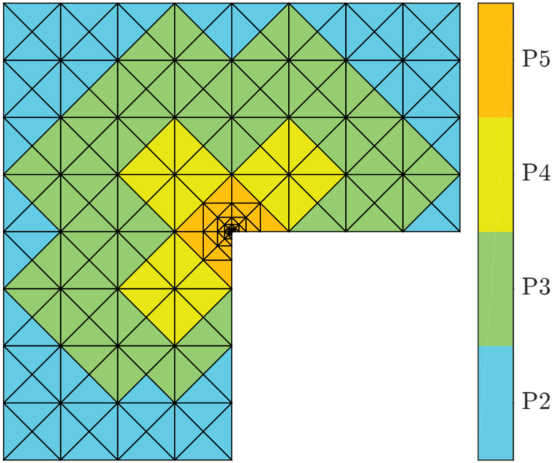

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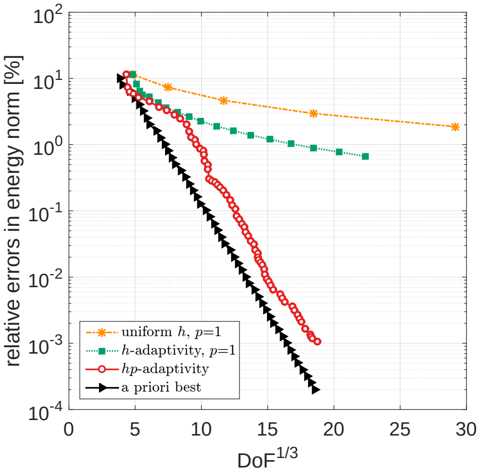

Relative error as a function of DoF

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- **total error estimate** on mesh $\mathcal{T}_\ell$, linearization step k, algebraic solver step i

$$\underbrace{\|u - u_\ell^{k,i}\|_*}_{\text{total error}} \leq \underbrace{\eta_{\ell,\mathrm{disc}}^{k,i}}_{\text{discretization estimate}} + \underbrace{\eta_{\ell,\mathrm{lin}}^{k,i}}_{\text{linearization estimate}} + \underbrace{\eta_{\ell,\mathrm{alg}}^{k,i}}_{\text{algebraic estimate}}$$

- **balancing error components**: work where needed

$\eta_{\ell,\mathrm{alg}}^{k,i} \leq \gamma_{\mathrm{alg}} \max\{\eta_{\ell,\mathrm{disc}}^{k,i}, \eta_{\ell,\mathrm{lin}}^{k,i}\}$	stopping criterion linear solver,
$\eta_{\ell,\mathrm{lin}}^{k,i} \leq \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i}$	stopping criterion nonlinear solver,
$\theta \eta_{\ell,\mathrm{disc}}^{k,i} \leq \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i}$	adaptive mesh refinement

- link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuflhard (1991), Eisenstat & Walker (1994)

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- Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)

Optimal error decay rate wrt overall computational cost

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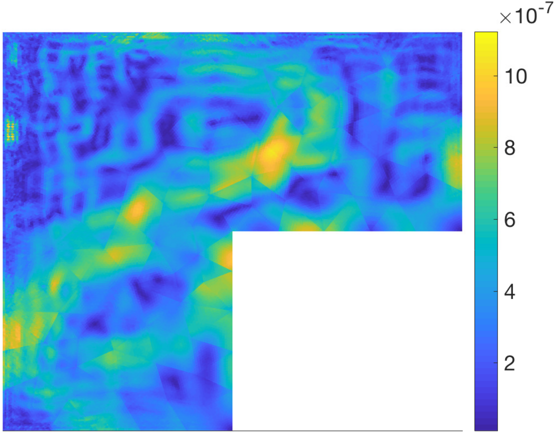
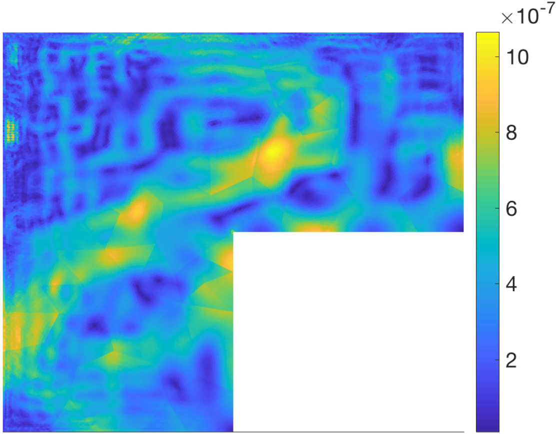


Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2017)

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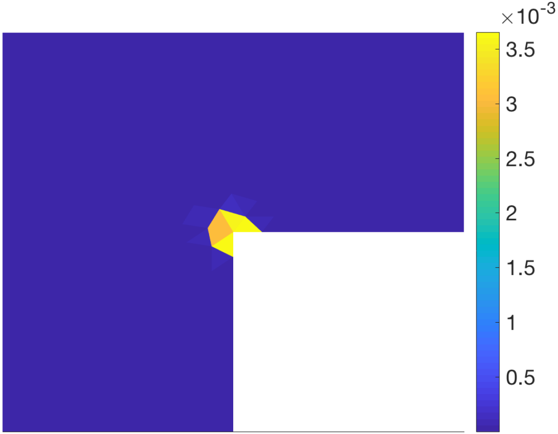
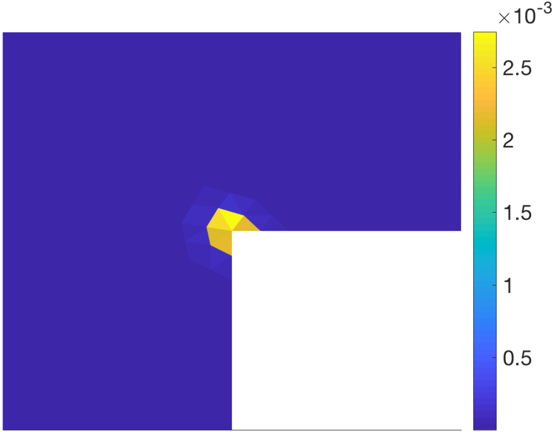


Estimated total errors $\eta_K(u_\ell^i)$



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J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, preprint (2017)

Nonlinear pb $-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$

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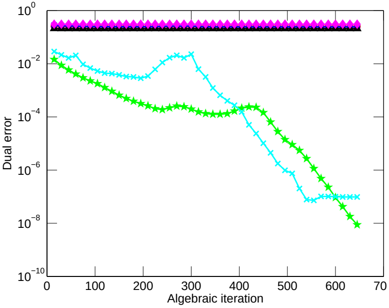
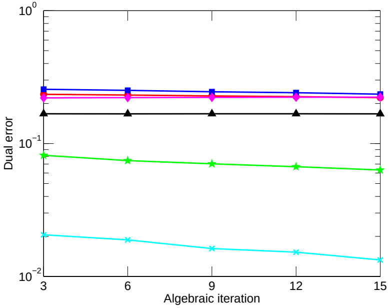
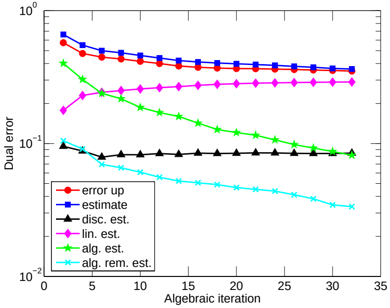


Newton



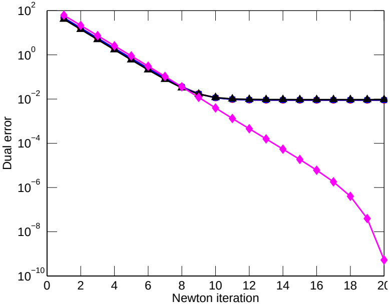
inexact Newton



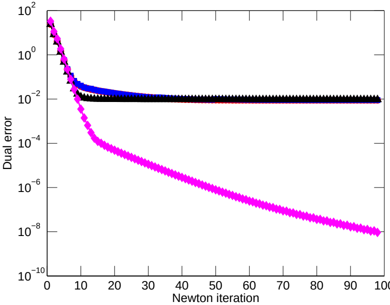
ad. inexact Newton

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Nonlinear pb $-\nabla\cdot\boldsymbol{\sigma}(\nabla u) = f$: including **linearization** and **algebraic** error: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$



Newton



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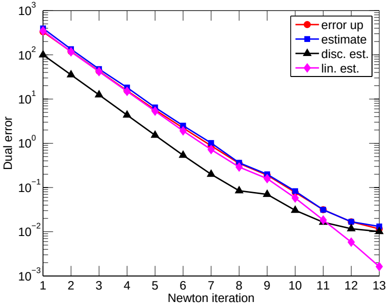

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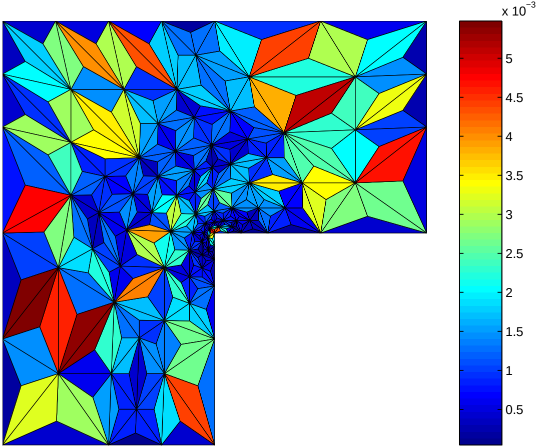
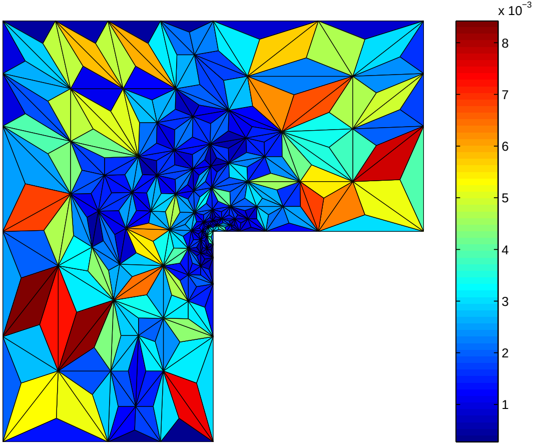


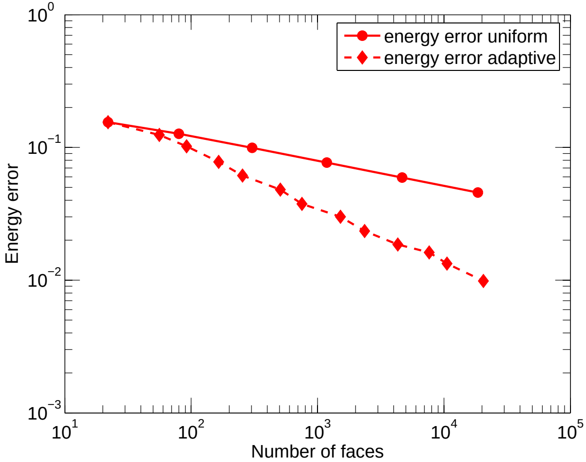
Estimated errors $\eta_K(u_\ell^{k,i})$



Exact errors $\|\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_\ell^{k,i})\|_{q,K}$

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

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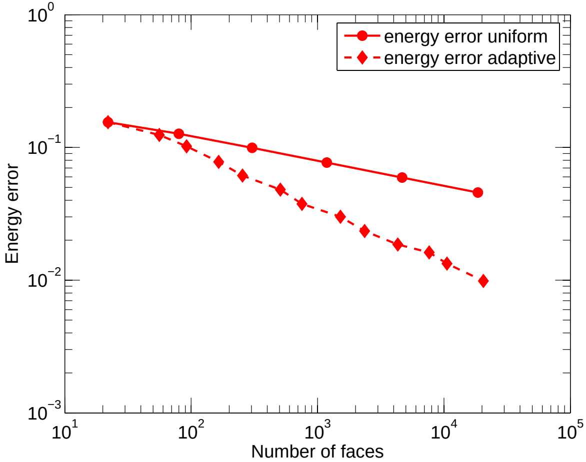

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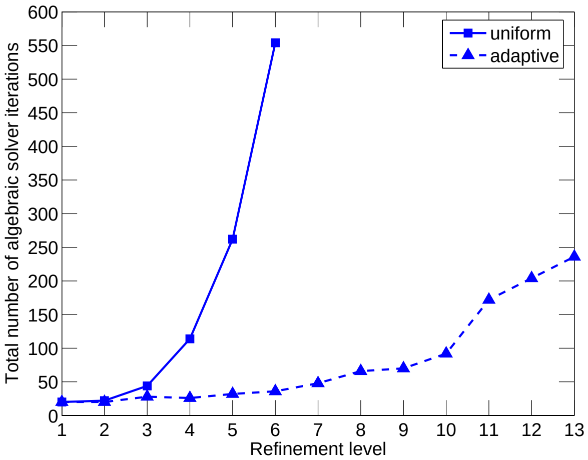
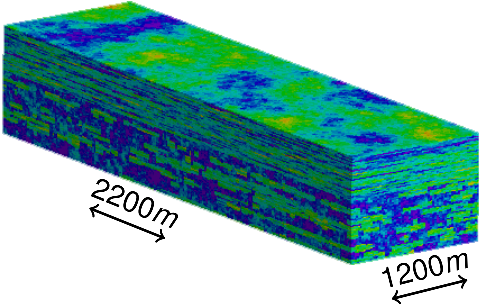


Optimal computational cost

A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2013)

Can we certify error in a practical case $-\nabla\cdot(\boldsymbol{K}\nabla u) = f$: outflow error $\left|\int_{y=2200} \boldsymbol{K}\nabla(u - u_\ell)\cdot\mathbf{n}\right|$ (**goal functional**)

no of unknowns	825	3300	13200
rel. error est.	46%	34%	24%



Underground reservoir,
10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2019)

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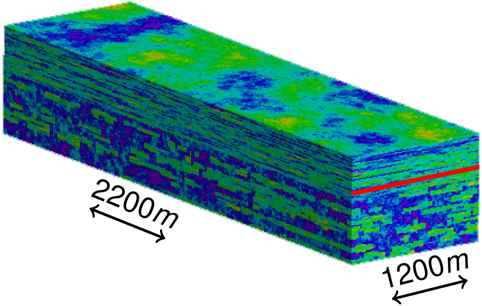

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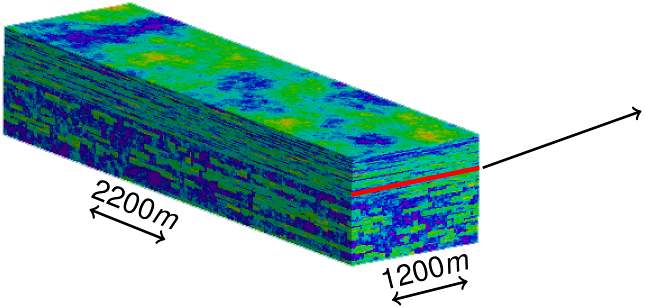
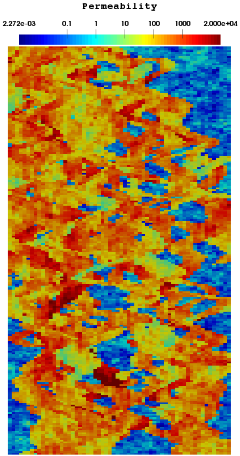


Underground reservoir, 10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2019)



Layer permeability

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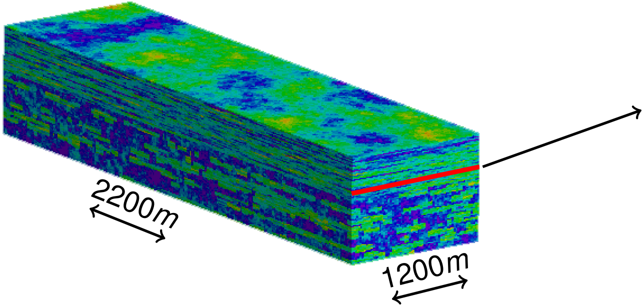

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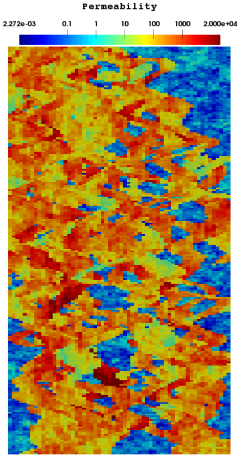

Layer permeability

Realistic environmental problem

Incompressible two-phase flow in porous media

Find *saturations* s_α and *pressures* p_α, $\alpha \in \{\mathrm{g}, \mathrm{w}\}$, such that

$$\begin{aligned} \partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\boldsymbol{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) &= q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\},\\ s_\mathrm{g} + s_\mathrm{w} &= 1,\\ p_\mathrm{g} - p_\mathrm{w} &= p_\mathrm{c}(s_\mathrm{w}) \end{aligned}$$

- unsteady, nonlinear, and degenerate problem
- coupled system of PDEs & algebraic constraints

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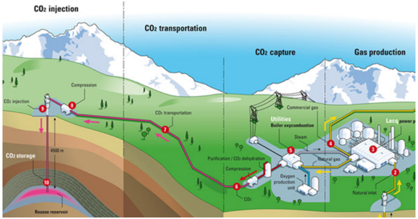
Carbon capture & geological storage



Space/time/nonlinear solver/linear solver adaptivity

movie

M. Vohralík, M.-F. Wheeler, Computational Geosciences (2013)

Outline

Laplace eigenvalue problem $-\Delta u = \lambda u$: theoretical results

A posteriori error estimates

1. *i*-th eigenvalue error

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

2. *i*-th eigenvector energy error

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

- **unified framework** for various numerical methods (planewaves, conforming/nonconforming/mixed/DG finite elements)
- taking into account **inexact solvers**
- extension to **multiple eigenvalues** and **clusters**
- extension to the **Gross–Pitaevskii** equation, balancing error components

Convergence and optimal error decay rate wrt degrees of freedom

Dai, Xu, Zhou (2008), Giani & Graham (2009), Gallistl (2015), Bonito & Demlow (2016)

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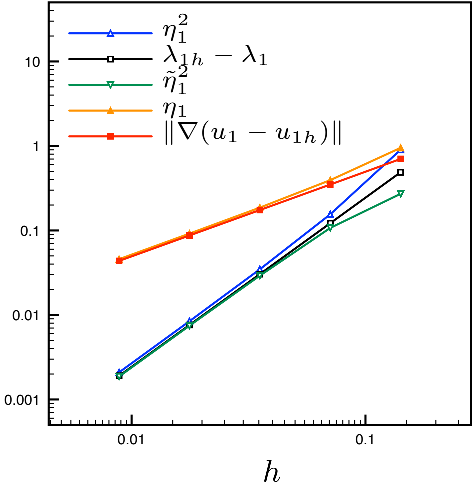
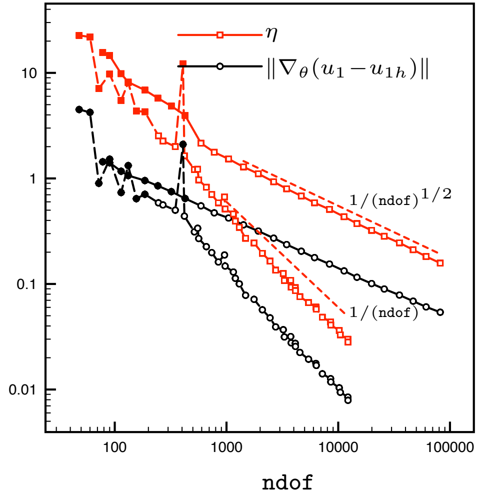
Bounds on eigenvalues and eigenvector errors, adaptivity



Unit square, conforming FEs, $p = 1$

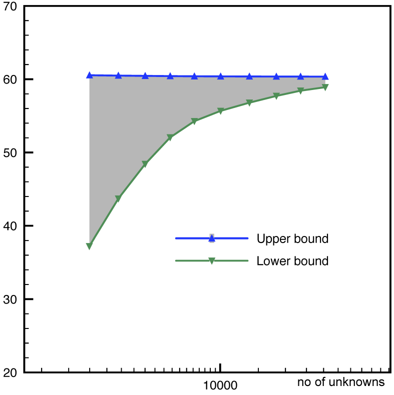


L-shape, adaptivity, DGs, $p = 1, 2$

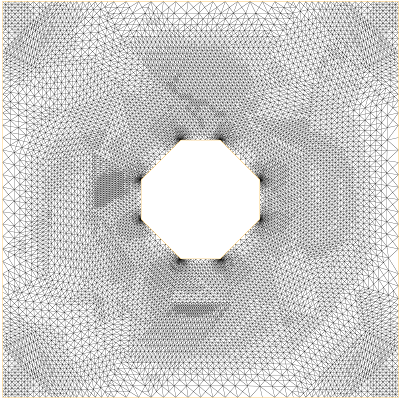
E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, Numerische Mathematik (2018)

Inclusion bounds on eigenvalues, adaptivity

no of unknowns	2494	3390	4508	7602	13640	18163	23494	30533
rel. error est.	48%	32%	22%	11%	6.1%	4.5%	3.2%	2.4%



First eigenvalue inclusion



Adaptively refined mesh

E. Cancès, G. Dusson, Y. Maday, B. Stamm, M. Vohralík, SIAM Journal on Numerical Analysis (2017)

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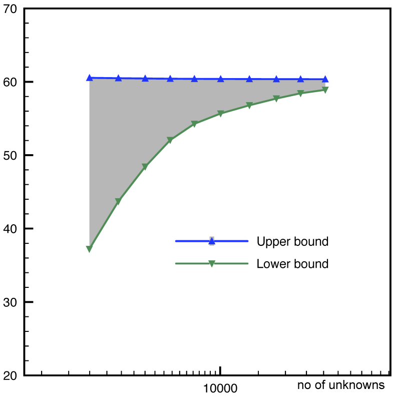

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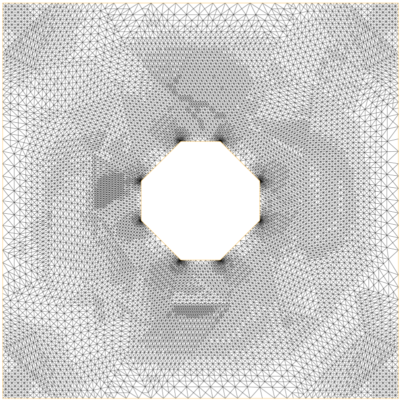

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Outline

Outlook

Work package 3

Thank you for your attention!

Outlook

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