

A posteriori error estimates and adaptive solvers for porous media flows

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European Research Council



Outline

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Introduction: context, motivation, and goals

2

Steady linear Darcy flow

- Discretization
- A posteriori error estimate
- Numerical experiments

3

Adaptivity: mesh, polynomial degree, linear solvers, nonlinear solvers

- Mesh and polynomial degree
- Linear and nonlinear solvers
- Error in a quantity of interest

4

Unsteady multi-phase multi-compositional Darcy flow

5

Conclusions

Context

Multi-phase, multi-compositional porous media flows

- **unsteady nonlinear** degenerate **systems** of PDEs
- possibly algebraic inequality constraints (phase appearance/disappearance)

General polygonal/polyhedral meshes, arbitrary scheme

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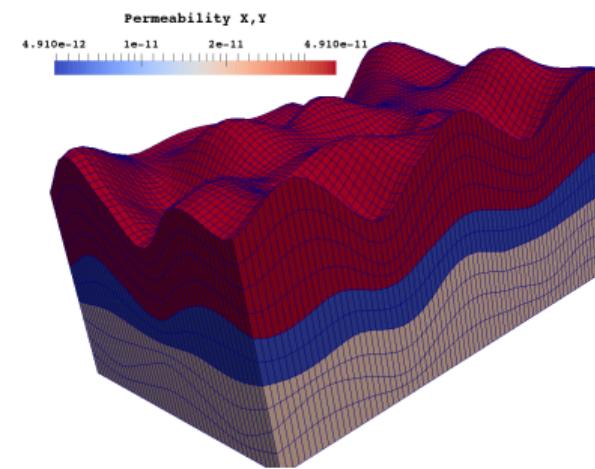
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Example: steady nonlinear Darcy flow $\nabla \cdot (-\underline{\mathbf{K}}(\nabla p)\nabla p) = f$

Discretization: system of nonlinear algebraic eqs

Find $\mathbf{P} \in \mathbb{R}^N$ such that

$$\underbrace{\mathcal{U}}_{\text{nonlin. op.}}(\mathbf{P}) = \mathbf{F}$$

Linearization: system of linear algebraic eqs

Find $\mathbf{P}^k \in \mathbb{R}^N$ such that

$$\underbrace{\mathbf{U}^{k-1}}_{\text{matrix}} \mathbf{P}^k = \mathbf{F}^{k-1}$$

Algebraic solver:

On step i , one has $\mathbf{P}^{k,i} \in \mathbb{R}^N$ such that

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Common situation

- **too costly** if $i, k \rightarrow \infty$
- **mass balance lost**
- **linearization stopping crit.**
 $\|\mathbf{P}^k - \mathbf{P}^{k-1}\|_\infty$ small,
algebraic stopping crit.
 $\|\mathbf{R}^{k,i}\|_2 / \|\mathbf{R}^{k,0}\|_2$ small:
comparing apples and oranges
- **no control of the overall error** between the obtained numerical approximation $\mathbf{P}^{k,i}$ and the exact solution \mathbf{p}

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$$\|\mathbf{u}|_{I_n} - \mathbf{u}_h^{n,k,i}\| \leq \eta_{\text{sp}}^{n,k,i} + \eta_{\text{tm}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}$$

- valid at each step: time n , linearization k , linear solver i
- distinguishing different error components, all estimators with the same (flux) physical units
- easy to code, fast to evaluate, cosy to use in practice
- full adaptivity (stopping criteria for linear and nonlinear solvers, mesh h/p refinement, time step adjustment)

Construction of the estimates interconnected with recovering mass balance at each step, e.g.

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Linear Darcy flow

Steady linear Darcy flow

$$\begin{aligned}-\nabla \cdot (\underline{\mathbf{K}} \nabla p) &= f && \text{in } \Omega, \\ p &= 0 && \text{on } \partial\Omega\end{aligned}$$

- $\Omega \subset \mathbb{R}^d$, $d \geq 1$, polytope
- $f \in L^2(\Omega)$ source term, pw constant for simplicity
- $\underline{\mathbf{K}} \in [L^\infty(\Omega)]^{d \times d}$ symmetric elliptic diffusion-dispersion tensor (pw constant)

Unknowns

- p pressure head
- $\mathbf{u} := -\underline{\mathbf{K}} \nabla p$ Darcy velocity (flux)

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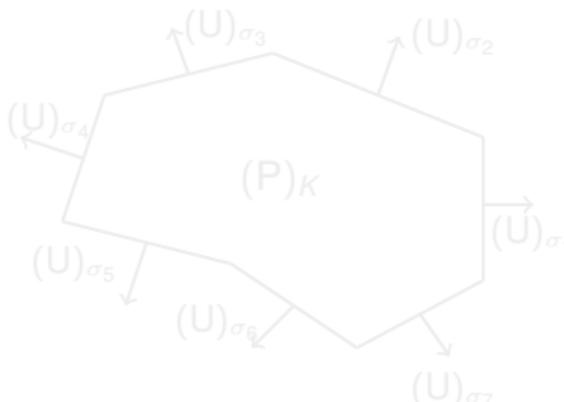
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Locally conservative discretization

Assumption A (Locally conservative discretization)

- ➊ There is one pressure $(P)_K \in \mathbb{R}$ per element $K \in \mathcal{T}_H$ and one face normal flux $(U)_\sigma \in \mathbb{R}$ per face $\sigma \in \mathcal{E}_H$.
- ➋ The flux balance is satisfied, with $(F)_K := (f, 1)_K$:

$$\sum_{\sigma \in \mathcal{E}_K} (U)_\sigma \mathbf{n}_{K,\sigma} \cdot \mathbf{n}_\sigma = (F)_K \quad \forall K \in \mathcal{T}_H.$$



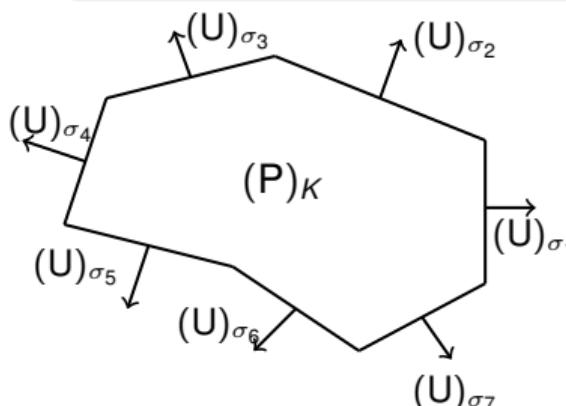
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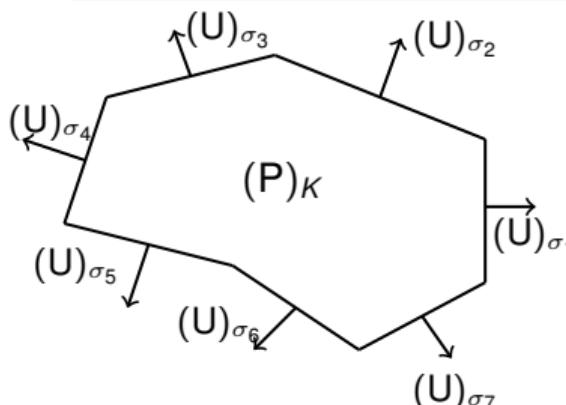
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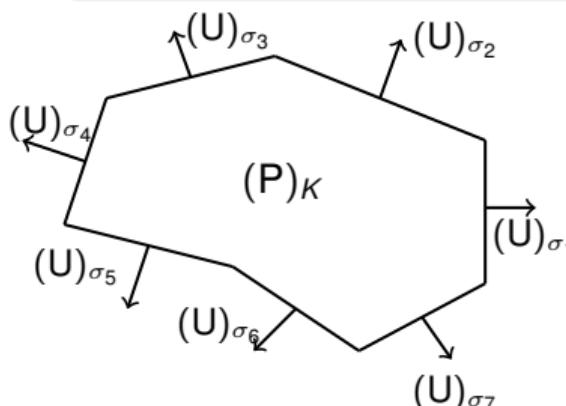
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A posteriori error estimate

Theorem (Linear Darcy flow)

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where

$$\begin{aligned} \eta_K^2 := & (\mathbf{U}_K^{\text{ext}})^t \mathbf{A}_K \mathbf{U}_K^{\text{ext}} + \mathbf{S}_K^t \mathbf{S}_K \mathbf{S}_K \\ & + 2(\mathbf{U}_K^{\text{ext}})^t \mathbf{S}_K^{\text{ext}} - 2(\mathbf{F})_K |K|^{-1} \mathbf{1}^t \mathbf{M}_K \mathbf{S}_K. \end{aligned}$$

Comments

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- \mathbf{A}_K , \mathbf{S}_K , \mathbf{M}_K : mass/stiffness matrices on element K
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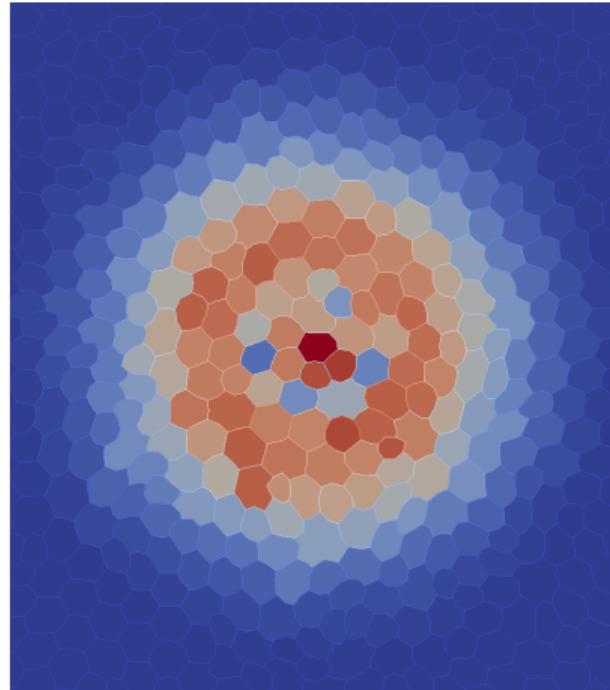
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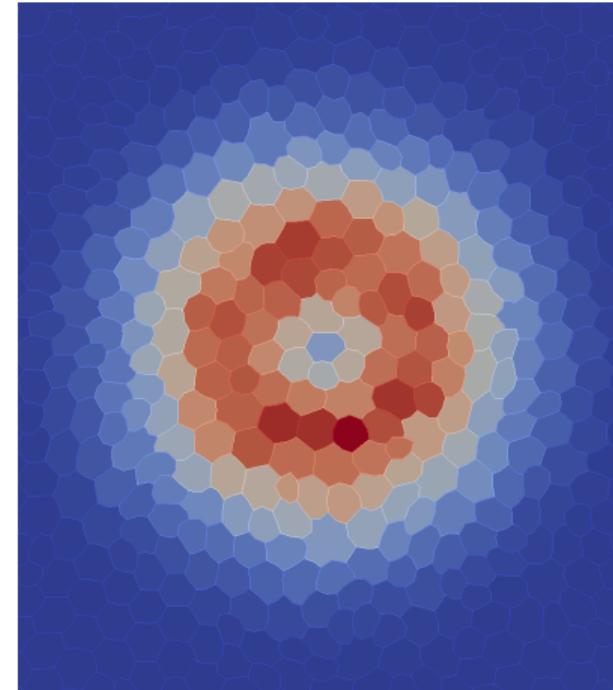
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Energy error & simple polygonal estimate



Estimated error distribution



Exact error distribution

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2020)



How large is the overall error?

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p\ }$ |
|-----------------|-----|-------------|---|-----------------------|--|
| h_0 | 1 | 1.25 | 28% | 1.07 | 24% |
| $\approx h_0/2$ | | | | | |
| $\approx h_0/4$ | | | | | |
| $\approx h_0/8$ | | | | | |

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

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p\ }$ | $\ p - p_h\ _{L^2}$ |
|-------|-----|-------------|--|-----------------------|---|---------------------|
| h_0 | 1 | 1.25 | 28% | 1.07 | 24% | 0.01 |

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

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p\ }$ | $F^h = \frac{\eta(p_h)}{\ \nabla(p - p_h)\ }$ |
|-------|-----|-------------|--|-----------------------|---|---|
| h_0 | 1 | 1.25 | 28% | 1.07 | 24% | 1.17 |

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

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p\ }$ | $F^{\text{eff}} = \frac{\eta(p_h)}{\ \nabla(p - p_h)\ }$ |
|--|-----|-----------------------|--|-----------------------|---|--|
| h_0 | 1 | 1.25 | 28% | 1.07 | 24% | 1.17 |
| $\approx h_0/2$ | | 6.07×10^{-1} | 14% | 5.56×10^{-1} | 14% | |
| $\approx h_0/4$ | | | | | | |
| $\approx h_0/8$ | | | | | | |
| $\approx h_0/16$ | | | | | | |
| $\approx h_0/32$ | | | | | | |
| $\approx h_0/64$ | | | | | | |
| $\approx h_0/128$ | | | | | | |
| $\approx h_0/256$ | | | | | | |
| $\approx h_0/512$ | | | | | | |
| $\approx h_0/1024$ | | | | | | |
| $\approx h_0/2048$ | | | | | | |
| $\approx h_0/4096$ | | | | | | |
| $\approx h_0/8192$ | | | | | | |
| $\approx h_0/16384$ | | | | | | |
| $\approx h_0/32768$ | | | | | | |
| $\approx h_0/65536$ | | | | | | |
| $\approx h_0/131072$ | | | | | | |
| $\approx h_0/262144$ | | | | | | |
| $\approx h_0/524288$ | | | | | | |
| $\approx h_0/1048576$ | | | | | | |
| $\approx h_0/2097152$ | | | | | | |
| $\approx h_0/4194304$ | | | | | | |
| $\approx h_0/8388608$ | | | | | | |
| $\approx h_0/16777216$ | | | | | | |
| $\approx h_0/33554432$ | | | | | | |
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How large is the overall error? (model pb, known sol.)

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p_h\ }$ | $J^{\text{eff}} = \frac{\eta(p_h)}{\ \nabla(p - p_h)\ }$ |
|--------------------------------------|-----|--|--|--|---|--|
| 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% | |
| $\approx h_0/4$ | | 3.10×10^{-1} | 7.0% | 2.92×10^{-1} | 6.6% | |
| $\approx h_0/8$ | | 1.45×10^{-1} | 3.5% | 1.39×10^{-1} | 3.1% | |
| $\approx h_0/16$ | | 6.22×10^{-2} | 1.7% | 6.22×10^{-2} | 1.7% | |
| $\approx h_0/32$ | | 3.11×10^{-2} | 0.9% | 3.11×10^{-2} | 0.9% | |
| $\approx h_0/64$ | | 1.55×10^{-2} | 0.4% | 1.55×10^{-2} | 0.4% | |
| $\approx h_0/128$ | | 7.77×10^{-3} | 0.2% | 7.77×10^{-3} | 0.2% | |
| $\approx h_0/256$ | | 3.90×10^{-3} | 0.1% | 3.90×10^{-3} | 0.1% | |
| $\approx h_0/512$ | | 1.95×10^{-3} | 0.05% | 1.95×10^{-3} | 0.05% | |
| $\approx h_0/1024$ | | 9.75×10^{-4} | 0.025% | 9.75×10^{-4} | 0.025% | |
| $\approx h_0/2048$ | | 4.87×10^{-4} | 0.01% | 4.87×10^{-4} | 0.01% | |
| $\approx h_0/4096$ | | 2.44×10^{-4} | 0.005% | 2.44×10^{-4} | 0.005% | |
| $\approx h_0/8192$ | | 1.22×10^{-4} | 0.0025% | 1.22×10^{-4} | 0.0025% | |
| $\approx h_0/16384$ | | 6.11×10^{-5} | 0.001% | 6.11×10^{-5} | 0.001% | |
| $\approx h_0/32768$ | | 3.05×10^{-5} | 0.0005% | 3.05×10^{-5} | 0.0005% | |
| $\approx h_0/65536$ | | 1.53×10^{-5} | 0.00025% | 1.53×10^{-5} | 0.00025% | |
| $\approx h_0/131072$ | | 7.66×10^{-6} | 0.000125% | 7.66×10^{-6} | 0.000125% | |
| $\approx h_0/262144$ | | 3.83×10^{-6} | 0.0000625% | 3.83×10^{-6} | 0.0000625% | |
| $\approx h_0/524288$ | | 1.91×10^{-6} | 0.00003125% | 1.91×10^{-6} | 0.00003125% | |
| $\approx h_0/1048576$ | | 9.55×10^{-7} | 0.000015625% | 9.55×10^{-7} | 0.000015625% | |
| $\approx h_0/2097152$ | | 4.77×10^{-7} | 0.0000078125% | 4.77×10^{-7} | 0.0000078125% | |
| $\approx h_0/4194304$ | | 2.38×10^{-7} | 0.00000390625% | 2.38×10^{-7} | 0.00000390625% | |
| $\approx h_0/8388608$ | | 1.19×10^{-7} | 0.000001953125% | 1.19×10^{-7} | 0.000001953125% | |
| $\approx h_0/16777216$ | | 5.95×10^{-8} | 0.0000009765625% | 5.95×10^{-8} | 0.0000009765625% | |
| $\approx h_0/33554432$ | | 2.98×10^{-8} | 0.00000048828125% | 2.98×10^{-8} | 0.00000048828125% | |
| $\approx h_0/67108864$ | | 1.49×10^{-8} | 0.000000244140625% | 1.49×10^{-8} | 0.000000244140625% | |
| $\approx h_0/134217728$ | | 7.45×10^{-9} | 0.0000001220703125% | 7.45×10^{-9} | 0.0000001220703125% | |
| $\approx h_0/268435456$ | | 3.73×10^{-9} | 0.00000006103515625% | 3.73×10^{-9} | 0.00000006103515625% | |
| $\approx h_0/536870912$ | | 1.86×10^{-9} | 0.000000030517578125% | 1.86×10^{-9} | 0.000000030517578125% | |
| $\approx h_0/1073741824$ | | 9.31×10^{-10} | 0.0000000152587890625% | 9.31×10^{-10} | 0.0000000152587890625% | |
| $\approx h_0/2147483648$ | | 4.65×10^{-10} | 0.00000000762939453125% | 4.65×10^{-10} | 0.00000000762939453125% | |
| $\approx h_0/4294967296$ | | 2.32×10^{-10} | 0.000000003814697265625% | 2.32×10^{-10} | 0.000000003814697265625% | |
| $\approx h_0/8589934592$ | | 1.16×10^{-10} | 0.0000000019073486328125% | 1.16×10^{-10} | 0.0000000019073486328125% | |
| $\approx h_0/17179869184$ | | 5.8×10^{-11} | 0.00000000095367431640625% | 5.8×10^{-11} | 0.00000000095367431640625% | |
| $\approx h_0/34359738368$ | | 2.9×10^{-11} | 0.000000000476837158203125% | 2.9×10^{-11} | 0.000000000476837158203125% | |
| $\approx h_0/68719476736$ | | 1.45×10^{-11} | 0.0000000002384185791015625% | 1.45×10^{-11} | 0.0000000002384185791015625% | |
| $\approx h_0/137438953472$ | | 7.25×10^{-12} | 0.00000000011920928955078125% | 7.25×10^{-12} | 0.00000000011920928955078125% | |
| $\approx h_0/274877906944$ | | 3.62×10^{-12} | 0.000000000059604644775390625% | 3.62×10^{-12} | 0.000000000059604644775390625% | |
| $\approx h_0/549755813888$ | | 1.81×10^{-12} | 0.0000000000298023223876953125% | 1.81×10^{-12} | 0.0000000000298023223876953125% | |
| $\approx h_0/1099511627776$ | | 9.05×10^{-13} | 0.00000000001490116119384765625% | 9.05×10^{-13} | 0.00000000001490116119384765625% | |
| $\approx h_0/2199023255552$ | | 4.52×10^{-13} | 0.000000000007450580596923828125% | 4.52×10^{-13} | 0.000000000007450580596923828125% | |
| $\approx h_0/4398046511104$ | | 2.26×10^{-13} | 0.0000000000037252902984619140625% | 2.26×10^{-13} | 0.0000000000037252902984619140625% | |
| $\approx h_0/8796093022208$ | | 1.13×10^{-13} | 0.0000000000018626451492309573125% | 1.13×10^{-13} | 0.0000000000018626451492309573125% | |
| $\approx h_0/17592186044416$ | | 5.65×10^{-14} | 0.00000000000093132257461547865625% | 5.65×10^{-14} | 0.00000000000093132257461547865625% | |
| $\approx h_0/35184372088832$ | | 2.82×10^{-14} | 0.0000000000004656612873077393125% | 2.82×10^{-14} | 0.0000000000004656612873077393125% | |
| $\approx h_0/70368744177664$ | | 1.41×10^{-14} | 0.00000000000023283064365386965625% | 1.41×10^{-14} | 0.00000000000023283064365386965625% | |
| $\approx h_0/140737488355328$ | | 7.05×10^{-15} | 0.000000000000116415321826934828125% | 7.05×10^{-15} | 0.000000000000116415321826934828125% | |
| $\approx h_0/281474976710656$ | | 3.53×10^{-15} | 0.0000000000000582076609134674140625% | 3.53×10^{-15} | 0.0000000000000582076609134674140625% | |
| $\approx h_0/562949953421312$ | | 1.76×10^{-15} | 0.00000000000002910383045673370703125% | 1.76×10^{-15} | 0.00000000000002910383045673370703125% | |
| $\approx h_0/1125899906842624$ | | 8.8×10^{-16} | 0.000000000000014551915228366853515625% | 8.8×10^{-16} | 0.000000000000014551915228366853515625% | |
| $\approx h_0/2251799813685248$ | | 4.4×10^{-16} | 0.000000000000007275957614183426753125% | 4.4×10^{-16} | 0.000000000000007275957614183426753125% | |
| $\approx h_0/4503599627370496$ | | 2.2×10^{-16} | 0.00000000000000363797880709171337515625% | 2.2×10^{-16} | 0.00000000000000363797880709171337515625% | |
| $\approx h_0/9007199254740992$ | | 1.1×10^{-16} | 0.00000000000000181898940354585668753125% | 1.1×10^{-16} | 0.00000000000000181898940354585668753125% | |
| $\approx h_0/18014398509481984$ | | 5.5×10^{-17} | 0.0000000000000009094947017729283437515625% | 5.5×10^{-17} | 0.0000000000000009094947017729283437515625% | |
| $\approx h_0/36028797018963968$ | | 2.75×10^{-17} | 0.0000000000000004547473508864641718753125% | 2.75×10^{-17} | 0.0000000000000004547473508864641718753125% | |
| $\approx h_0/72057594037927936$ | | 1.375×10^{-17} | 0.00000000000000022737367544323208593753125% | 1.375×10^{-17} | 0.00000000000000022737367544323208593753125% | |
| $\approx h_0/14411518807585968$ | | 6.875×10^{-18} | 0.000000000000000113686837721616042968753125% | 6.875×10^{-18} | 0.000000000000000113686837721616042968753125% | |
| $\approx h_0/28823037615171936$ | | 3.4375×10^{-18} | 0.00000000000000056843418860880821488753125% | 3.4375×10^{-18} | 0.00000000000000056843418860880821488753125% | |
| $\approx h_0/57646075230343872$ | | 1.71875×10^{-18} | 0.000000000000000284217094304404107443753125% | 1.71875×10^{-18} | 0.000000000000000284217094304404107443753125% | |
| $\approx h_0/115292150460687744$ | | 8.59375×10^{-19} | 0.0000000000000001421085471522020537218753125% | 8.59375×10^{-19} | 0.0000000000000001421085471522020537218753125% | |
| $\approx h_0/230584300921375488$ | | 4.296875×10^{-19} | 0.0000000000000007105427357611012786093753125% | 4.296875×10^{-19} | 0.0000000000000007105427357611012786093753125% | |
| $\approx h_0/461168601842750976$ | | $2.1484375 \times 10^{-19}$ | 0.000000000000000355271367880550639304753125% | $2.1484375 \times 10^{-19}$ | 0.000000000000000355271367880550639304753125% | |
| $\approx h_0/922337203685501952$ | | $1.07421875 \times 10^{-19}$ | 0.0000000000000001776352739402751696523753125% | $1.07421875 \times 10^{-19}$ | 0.0000000000000001776352739402751696523753125% | |
| $\approx h_0/184467440737000384$ | | $5.37109375 \times 10^{-20}$ | 0.00000000000000008881763697013758488118753125% | $5.37109375 \times 10^{-20}$ | 0.00000000000000008881763697013758488118753125% | |
| $\approx h_0/368934881474000768$ | | $2.685546875 \times 10^{-20}$ | 0.000000000000000044408818485068792440593753125% | $2.685546875 \times 10^{-20}$ | 0.000000000000000044408818485068792440593753125% | |
| $\approx h_0/737869762948001536$ | | $1.3427734375 \times 10^{-20}$ | 0.00000000000000002220440924251438688229753125% | $1.3427734375 \times 10^{-20}$ | 0.00000000000000002220440924251438688229753125% | |
| $\approx h_0/1475739525896003072$ | | $6.7138671875 \times 10^{-21}$ | 0.0000000000000000111022046212571917644493753125% | $6.7138671875 \times 10^{-21}$ | 0.0000000000000000111022046212571917644493753125% | |
| $\approx h_0/2951479051792006144$ | | $3.35693359375 \times 10^{-21}$ | 0.000000000000000005551102305628598382894753125% | $3.35693359375 \times 10^{-21}$ | 0.000000000000000005551102305628598382894753125% | |
| $\approx h_0/5902958103584012288$ | | $1.678466796875 \times 10^{-21}$ | 0.00000000000000000277555115281429919144753125% | $1.678466796875 \times 10^{-21}$ | 0.00000000000000000277555115281429919144753125% | |
| $\approx h_0/11805916207168024576$ | | $8.392333984375 \times 10^{-22}$ | 0.000000000000000001387775576407149595724753125% | $8.392333984375 \times 10^{-22}$ | 0.000000000000000001387775576407149595724753125% | |
| $\approx h_0/23611832414336049152$ | | $4.1961669921875 \times 10^{-22}$ | 0.0000000000000000006938877882035747985624753125% | $4.1961669921875 \times 10^{-22}$ | 0.0000000000000000006938877882035747985624753125% | |
| $\approx h_0/47223664828672098304$ | | $2.09808349609375 \times 10^{-22}$ | 0.000000000000000000346943894101787399124753125% | $2.09808349609375 \times 10^{-22}$ | 0.000000000000000000346943894101787399124753125% | |
| $\approx h_0/94447329657344196608$ | | $1.049041748046875 \times 10^{-22}$ | 0.0000000000000000001734719470508936995624753125% | $1.049041748046875 \times 10^{-22}$ | 0.0000000000000000001734719470508936995624753125% | |
| $\approx h_0/188894659314688393216$ | | $5.245208740234375 \times 10^{-23}$ | 0.00000000000000000008673597352544684978124753125% | $5.245208740234375 \times 10^{-23}$ | 0.00000000000000000008673597352544684978124753125% | |
| $\approx h_0/377789318629376786432$ | | $2.6226043701171875 \times 10^{-23}$ | 0.000000000000000000043367986762723424890624753125% | $2.6226043701171875 \times 10^{-23}$ | 0.000000000000000000043367986762723424890624753125% | |
| $\approx h_0/755578637258753572864$ | | $1.31130218505859375 \times 10^{-23}$ | 0.0000000000000000000216839933813417124493124753125% | $1.31130218505859375 \times 10^{-23}$ | 0.0000000000000000000216839933813417124493124753125% | |
| $\approx h_0/1511157274517567145728$ | | $6.55651092529296875 \times 10^{-24}$ | 0.00000000000000000001084199669067085622468124753125% | $6.55651092529296875 \times 10^{-24}$ | 0.00000000000000000001084199669067085622468124753125% | |
| $\approx h_0/3022314549035134291456$ | | $3.278255462646484375 \times 10^{-24}$ | 0.00000000000000000005416998345134178311236124753125% | $3.278255462646484375 \times 10^{-24}$ | 0.00000000000000000005416998345134178311236124753125% | |
| $\approx h_0/6044629098070268$ | | | | | | |

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

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p_h\ }$ | $I^{\text{eff}} = \frac{\eta(p_h)}{\ \nabla(p - p_h)\ }$ |
|-------------------|-----|-----------------------|--|-----------------------|---|--|
| 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 |
| $\approx h_0/16$ | | 6.22×10^{-2} | 1.6% | 4.07×10^{-2} | 1.2% | 1.02 |
| $\approx h_0/32$ | | 2.99×10^{-2} | 0.8% | 2.03×10^{-2} | 0.6% | 1.01 |
| $\approx h_0/64$ | | 1.49×10^{-2} | 0.4% | 1.01×10^{-2} | 0.3% | 1.00 |
| $\approx h_0/128$ | | 6.25×10^{-3} | 0.2% | 4.99×10^{-3} | 0.2% | 1.00 |

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

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| $\approx h_0/8$ | | 1.45×10^{-1} | 3.3% | 1.39×10^{-1} | 3.1% | 1.04 |
| $\approx h_0/16$ | 2 | 4.23×10^{-2} | 9.5 $\times 10^{-3}\%$ | 4.07×10^{-2} | 9.2 $\times 10^{-3}\%$ | 1.04 |
| $\approx h_0/32$ | | | | | | |
| $\approx h_0/64$ | | | | | | |

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

| h | m | $\eta(p_h)$ | rel. error estimate $\frac{\eta(p_h)}{\ \nabla p_h\ }$ | $\ \nabla(p - p_h)\ $ | rel. error $\frac{\ \nabla(p - p_h)\ }{\ \nabla p_h\ }$ | $I^{\text{eff}} = \frac{\eta(p_h)}{\ \nabla(p - p_h)\ }$ |
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| $\approx h_0/8$ | | 1.45×10^{-1} | 3.3% | 1.39×10^{-1} | 3.1% | 1.04 |
| $\approx h_0/16$ | 2 | 4.23×10^{-2} | 9.5 $\times 10^{-3}\%$ | 4.07×10^{-2} | 9.2 $\times 10^{-3}\%$ | 1.04 |
| $\approx h_0/32$ | 3 | 2.62×10^{-2} | 5.9 $\times 10^{-3}\%$ | 2.60×10^{-2} | 5.9 $\times 10^{-3}\%$ | 1.01 |
| $\approx h_0/64$ | | 1.30×10^{-2} | 2.9 $\times 10^{-3}\%$ | 1.30×10^{-2} | 2.9 $\times 10^{-3}\%$ | 1.01 |

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

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| $\approx h_0/8$ | 4 | 1.45×10^{-1} | 3.3% | 1.39×10^{-1} | 3.1% | 1.04 |
| $\approx h_0/2$ | 2 | 4.23×10^{-2} | $9.5 \times 10^{-3}\%$ | 4.07×10^{-2} | $9.2 \times 10^{-3}\%$ | 1.04 |
| $\approx h_0/4$ | 3 | 2.62×10^{-3} | $5.9 \times 10^{-4}\%$ | 2.60×10^{-3} | $5.9 \times 10^{-4}\%$ | 1.01 |
| $\approx h_0/8$ | 4 | 2.60×10^{-7} | $5.9 \times 10^{-7}\%$ | 2.58×10^{-7} | $5.8 \times 10^{-7}\%$ | 1.01 |

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

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A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)

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

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| $\approx h_0/4$ | 3 | 2.62×10^{-4} | $5.9 \times 10^{-3}\%$ | 2.60×10^{-4} | $5.9 \times 10^{-3}\%$ | 1.01 |
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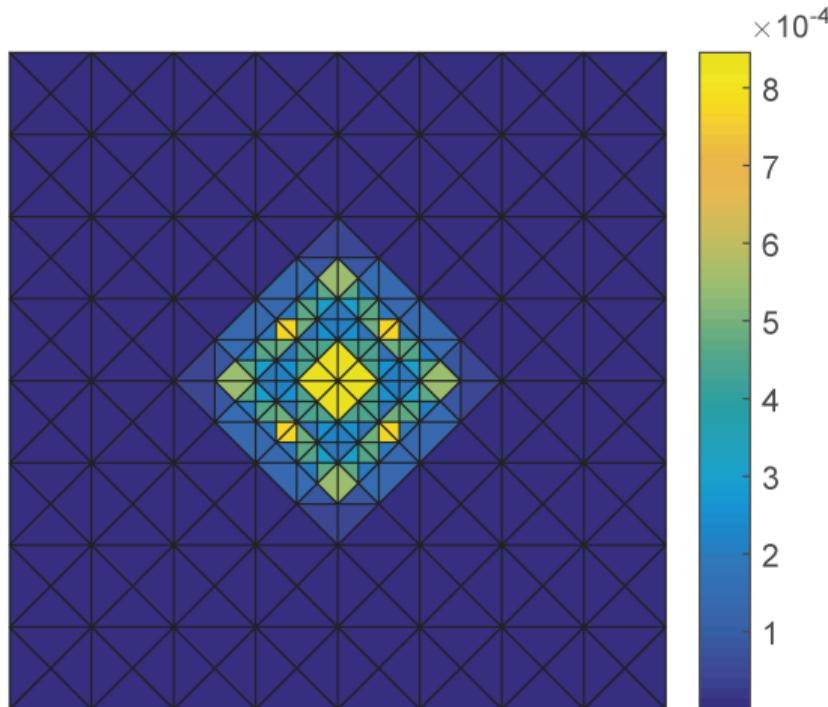
Outline

- 1 Introduction: context, motivation, and goals
- 2 Steady linear Darcy flow
 - Discretization
 - A posteriori error estimate
 - Numerical experiments
- 3 Adaptivity: mesh, polynomial degree, linear solvers, nonlinear solvers
 - Mesh and polynomial degree
 - Linear and nonlinear solvers
 - Error in a quantity of interest
- 4 Unsteady multi-phase multi-compositional Darcy flow
- 5 Conclusions

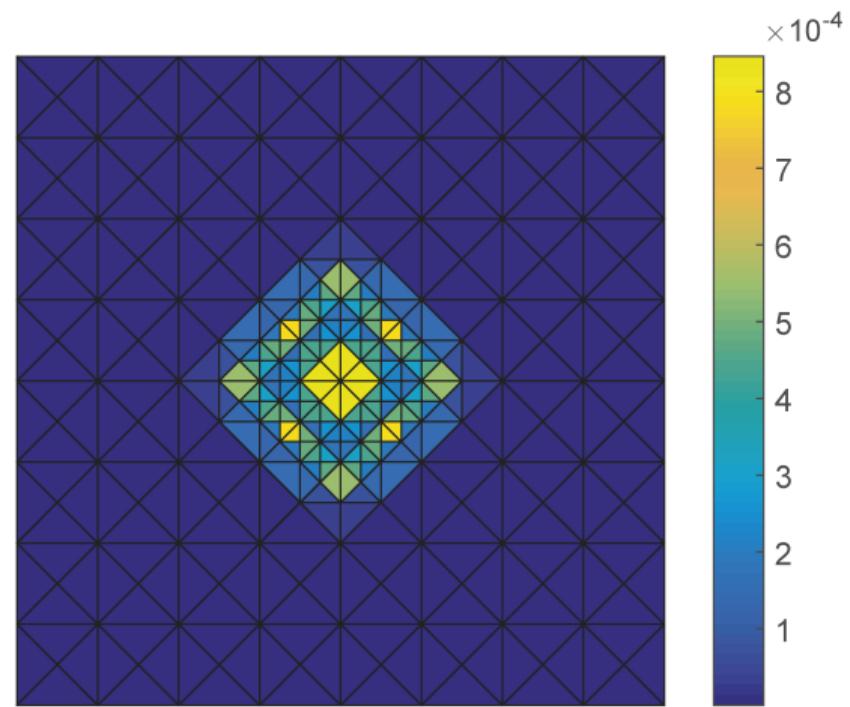
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Where (in space) is the error localized?



Estimated error distribution $\eta_K(p_h)$



Exact error distribution $\|\nabla(p - p_h)\|_K$

Adaptive mesh refinement (linear problem with exact solvers)

Adaptive mesh refinement

- Dörfler marking: subset \mathcal{M}_ℓ containing θ -fraction of the estimated error

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

Convergence on a sequence of adaptively refined meshes

- $\|\nabla(p - p_\ell)\| \rightarrow 0$
- 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

- $\|\nabla(p - p_\ell)\| \lesssim |\text{DoF}_\ell|^{-m/d}$ (replaces h^m)
- 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
- Morin, Nochetto, Siebert (2000), Stevenson (2005, 2007), Cascón, Kreuzer, Nochetto, Siebert (2008), Canuto, Nochetto, Stevenson, Verani (2017)

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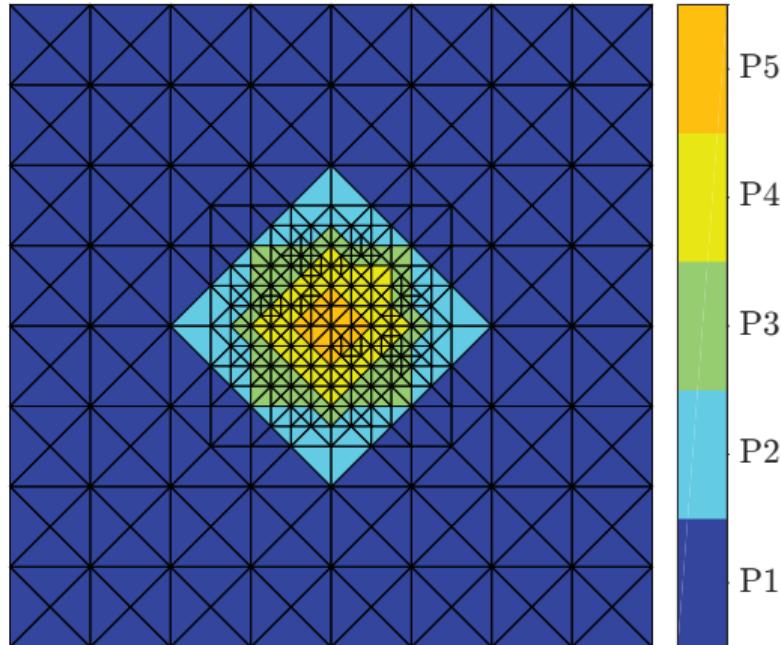
Convergence on a sequence of adaptively refined meshes

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Optimal error decay rate wrt degrees of freedom

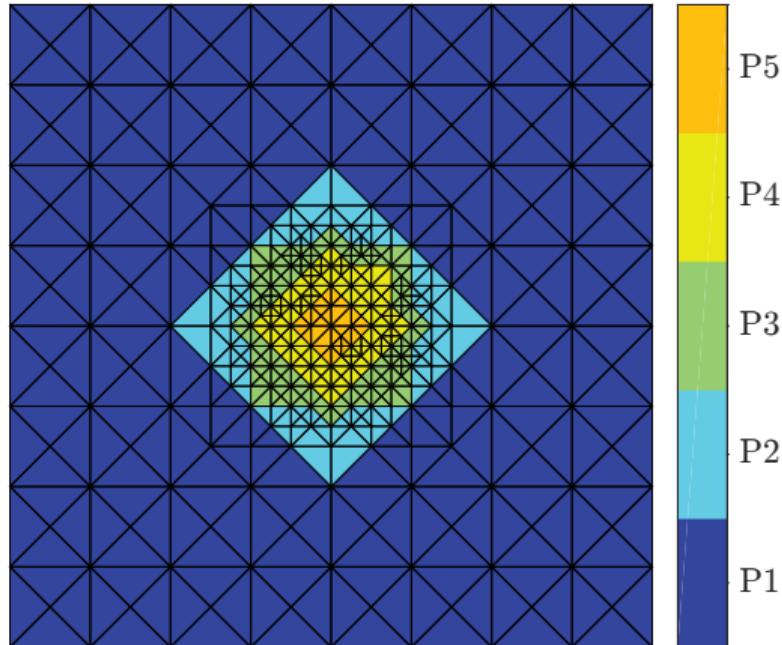
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Can we decrease the error efficiently? *hp* adaptivity, (**smooth** solution)

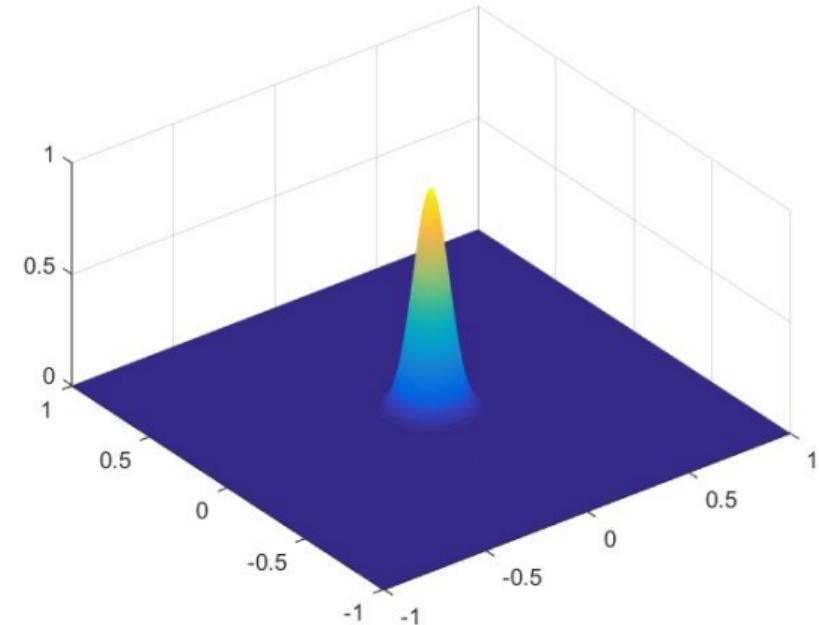


Mesh \mathcal{T}_ℓ and pol. degrees m_K

Can we decrease the error efficiently? *hp* adaptivity, (**smooth** solution)

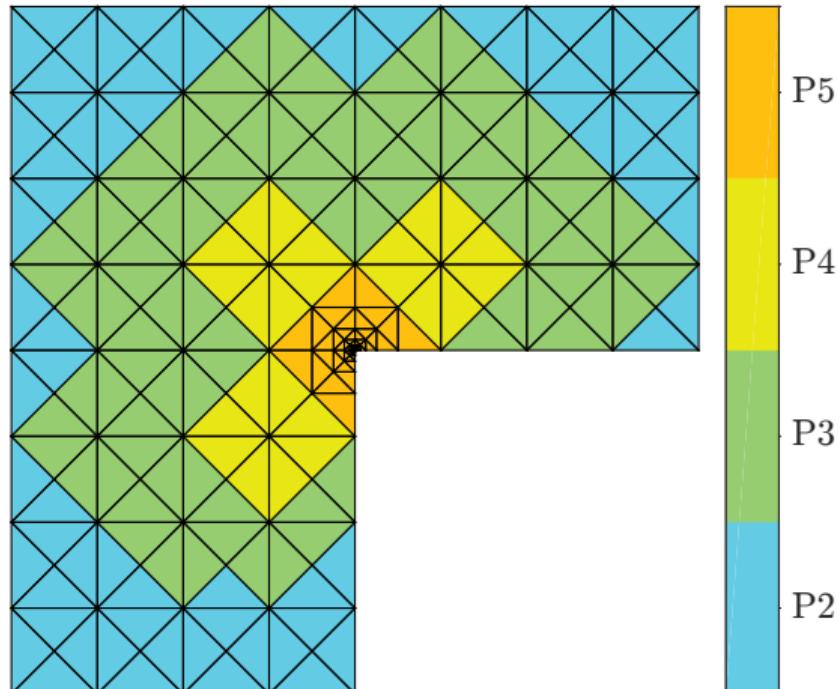


Mesh \mathcal{T}_ℓ and pol. degrees m_K



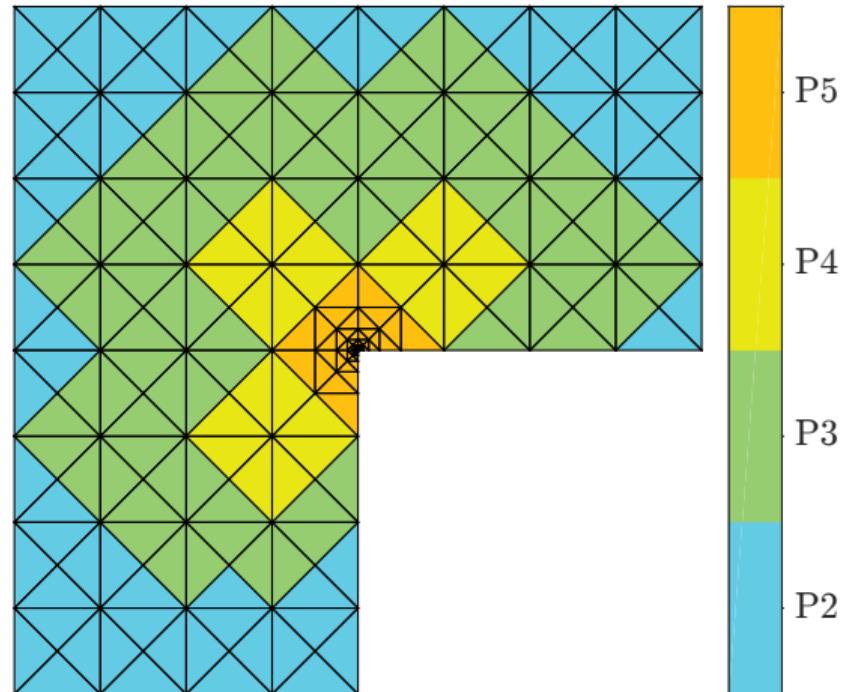
Exact solution

Can we decrease the error efficiently? *hp* adaptivity, (**singular** solution)

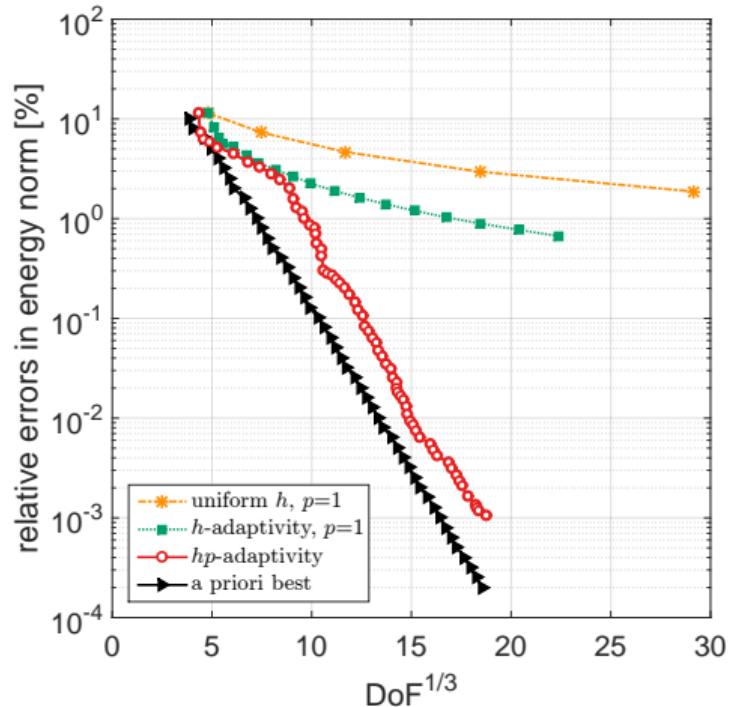


Mesh \mathcal{T}_ℓ and polynomial degrees m_K

Can we decrease the error efficiently? *hp* adaptivity, (**singular** solution)



Mesh T_ℓ and polynomial degrees m_K



Relative error as a function of DoF

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Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm

- total error estimate on mesh T_ℓ , linearization step k , algebraic solver step i

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

- balancing error components: work where needed

$$\eta_{\ell,\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \quad \eta_{\ell,\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \quad \text{stopping criterion linear solver}$$

$\gamma_{\text{alg}}, \gamma_{\text{lin}} < 1$ (e.g. $\gamma_{\text{alg}} = 10^{-3}$, $\gamma_{\text{lin}} = 10^{-4}$)

Adaptive refinement based on local error estimates

Adaptive refinement based on local error estimates

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

Convergence, optimal error decay rate wrt DoFs

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

Optimal error decay rate wrt overall computational cost

- Haberl, Praetorius, Schimanko, & Vohralík (preprint, 2020)

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- total error estimate on mesh \mathcal{T}_ℓ , linearization step k , algebraic solver step i

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

- balancing error components: work where needed

$$\eta_{\ell,\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \quad \eta_{\ell,\text{lin}}^{k,i} \quad \text{stopping criterion linear solver}$$

• γ_{alg} is a parameter that controls the accuracy of the linear solver
 • $\gamma_{\text{alg}} = 10^{-3}$ is a good choice for most problems

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

Convergence, optimal error decay rate wrt DoFs

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

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

$$\eta_{\ell,\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \max\{\eta_{\ell,\text{disc}}^{k,i}, \eta_{\ell,\text{lin}}^{k,i}\} \quad \text{stopping criterion linear solver,}$$

$$\eta_{\ell,\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i} \quad \text{stopping criterion nonlinear solver,}$$

$$\theta \eta_{\ell,\text{disc}}^{k,i} \leq \eta_{\text{disc},\mathcal{M}_\ell}^{k,i} \quad \text{adaptive mesh refinement}$$

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

Convergence, optimal error decay rate wrt DoFs

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

Optimal convergence rates for all components

- Haberl, Frey, & Vohralík (preprint, 2020)

Balancing error components (nonlinear problem with inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- total error estimate on mesh T_ℓ , linearization step k , algebraic solver step i

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

- balancing error components: work where needed

$$\eta_{\ell,\text{alg}}^{k,i} \leq \gamma_{\text{alg}} \max\{\eta_{\ell,\text{disc}}^{k,i}, \eta_{\ell,\text{lin}}^{k,i}\} \quad \text{stopping criterion linear solver,}$$

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

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

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

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

Convergence, optimal **error decay rate** wrt **DoFs**

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

Optimal error decay rate wrt **overall computational cost**

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$$\eta_{\ell,\text{lin}}^{k,i} \leq \gamma_{\text{lin}} \eta_{\text{disc}}^{k,i} \quad \text{stopping criterion nonlinear solver,}$$

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

Convergence, optimal error decay rate wrt DoFs

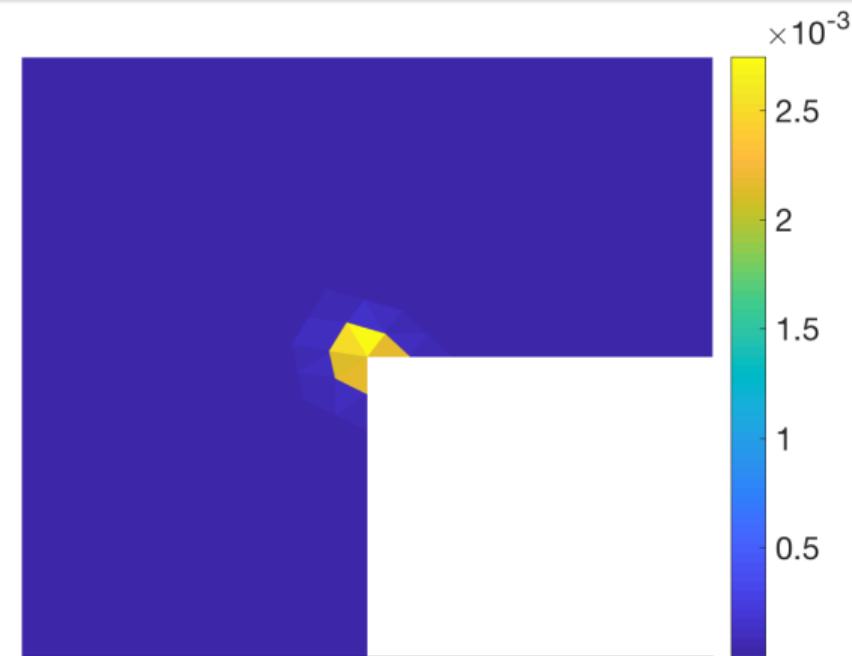
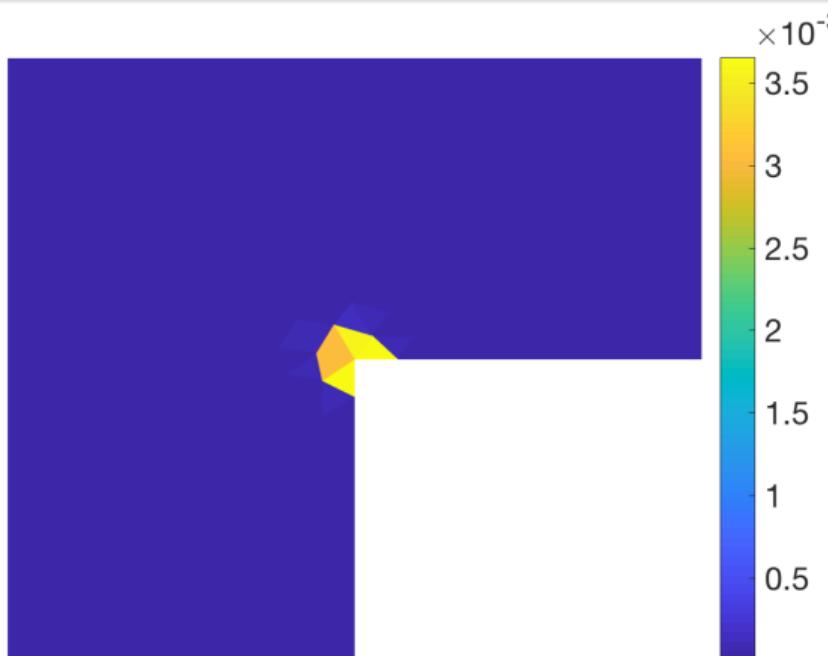
- Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)

Optimal error decay rate wrt overall computational cost

- Haberl, Praetorius, Schimanko, & Vohralík (preprint, 2020)

Including algebraic error: $\mathbb{U}_\ell \mathbf{P}_\ell^i \neq \mathbf{F}_\ell$

Including algebraic error: $\mathbb{U}_\ell \mathbf{P}_\ell^i \neq \mathbf{F}_\ell$

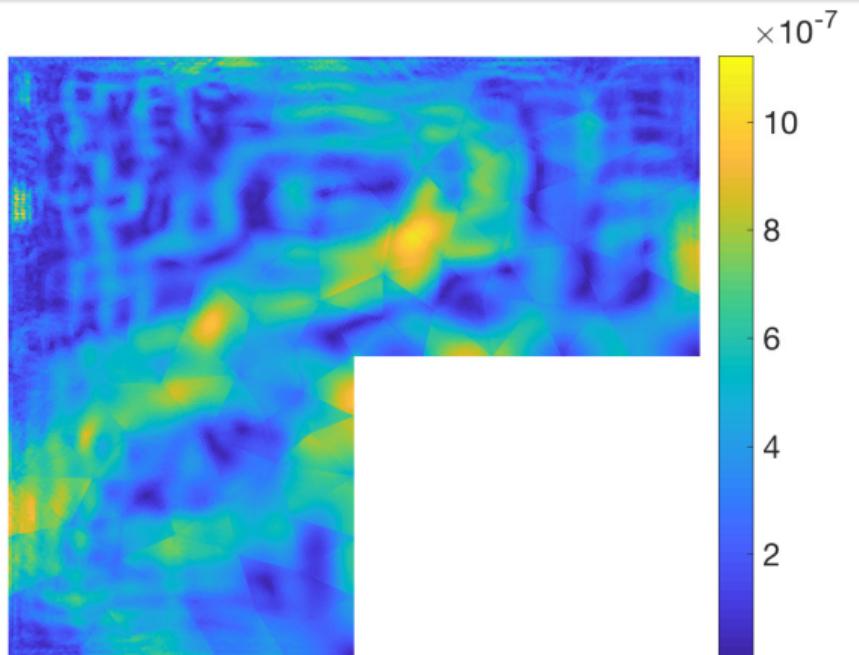


Estimated total errors $\eta_K(p_\ell^i)$

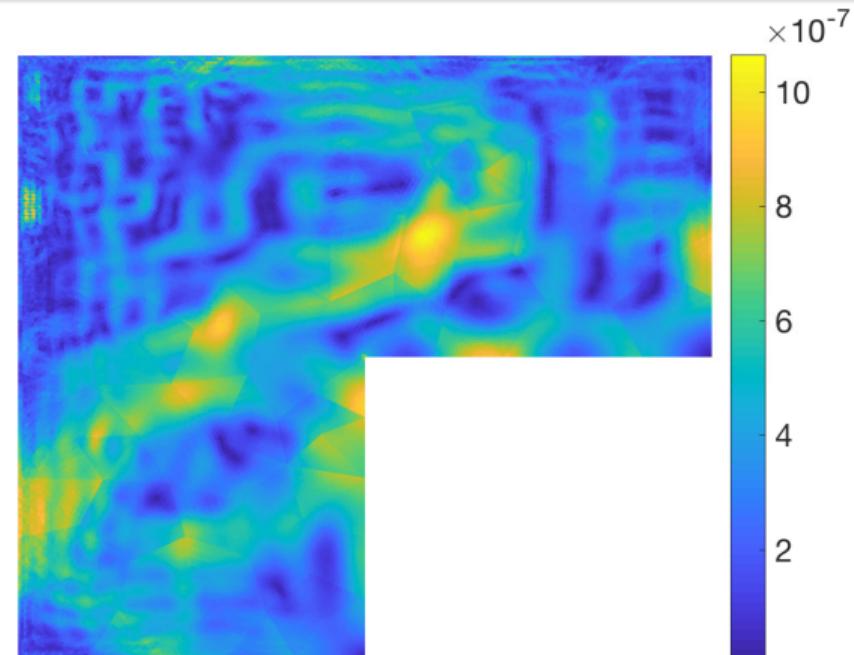
Exact total errors $\|\nabla(p - p_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

Including algebraic error: $\mathbb{U}_\ell \mathbf{P}_\ell^i \neq \mathbf{F}_\ell$



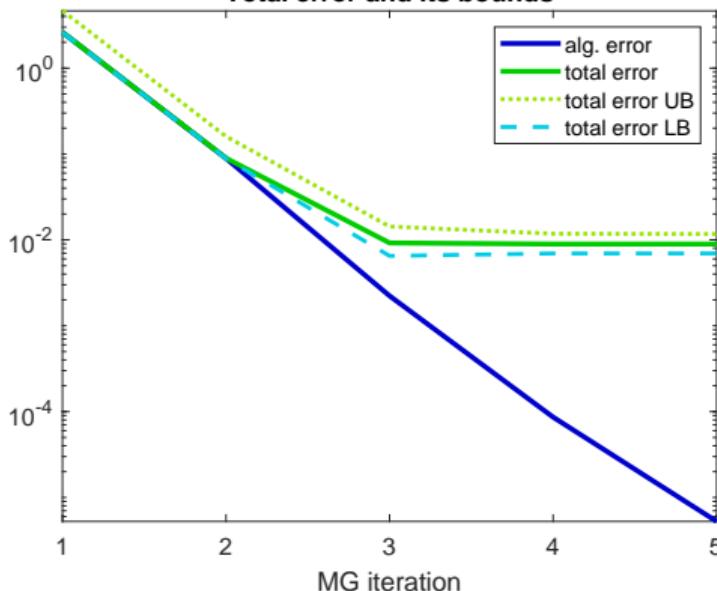
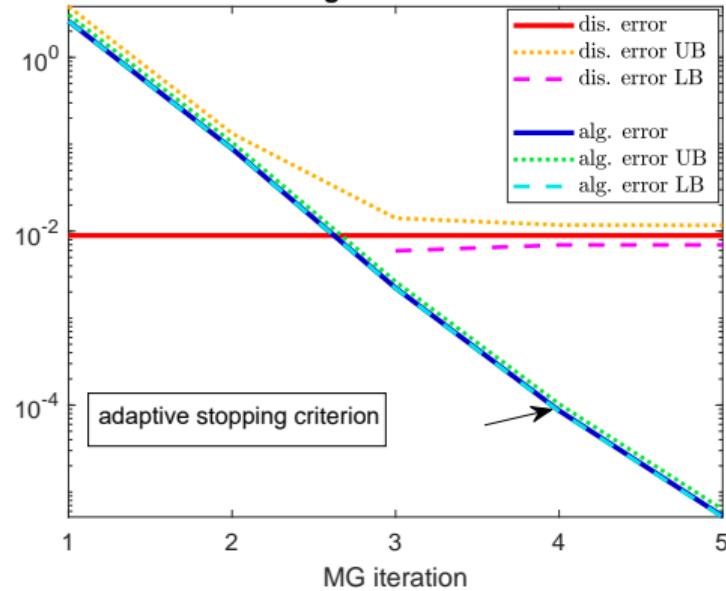
Estimated algebraic errors $\eta_{\text{alg}, \kappa}(p_\ell^i)$



Exact algebraic errors $\|\nabla(p_\ell - p_\ell^i)\|_\kappa$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

Including algebraic error: $\mathbb{U}_\ell \mathbf{P}_\ell^i \neq \mathbf{F}_\ell$

Total error and its bounds**Total error****Discretization and algebraic errors and their bounds****Error components and adaptive st. crit.**

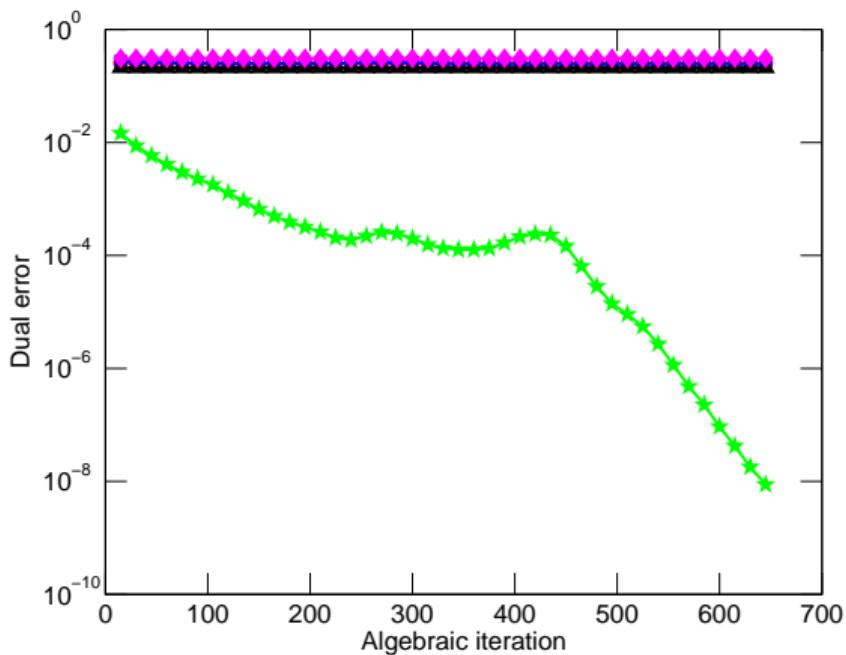
J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth (2020)

Nonlinear pb $-\nabla \cdot \sigma(\nabla p) = f$: including linearization and algebraic error: $\mathcal{U}_f(P_f) = F_f, U_f^{k-1}P_f = P_f^{k-1}$

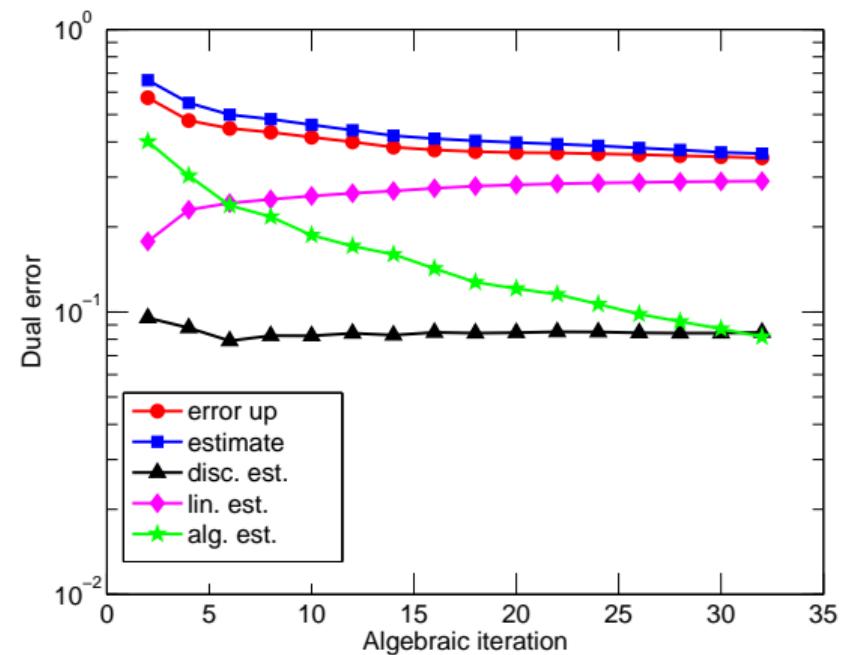
Nonlinear pb $-\nabla \cdot \sigma(\nabla p) = f$: including **linearization** and **algebraic error**: $\mathcal{U}_\ell(P_\ell^{k,i}) \neq F_\ell$, $U_\ell^{k-1}P_\ell = F_\ell^{k-1}$

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

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



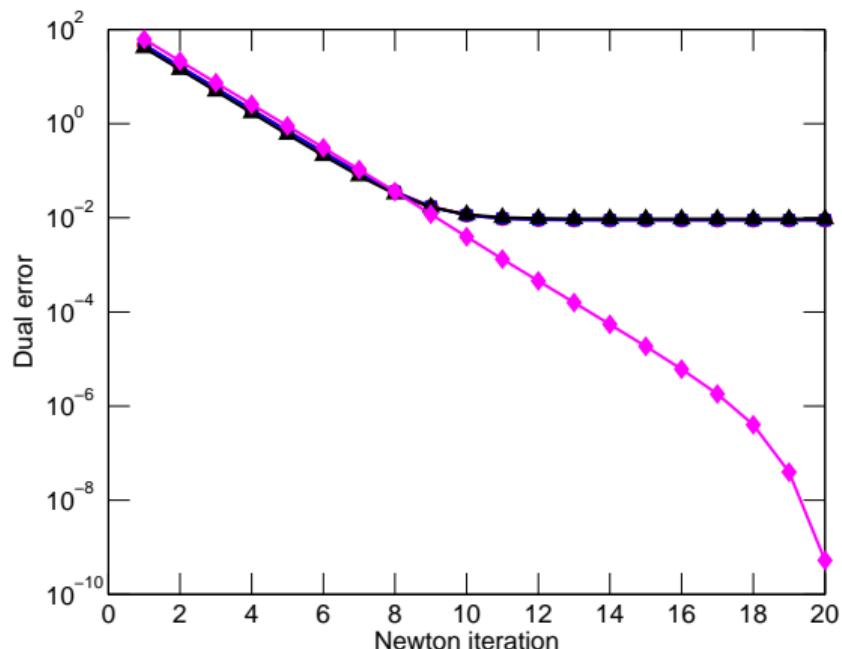
Newton



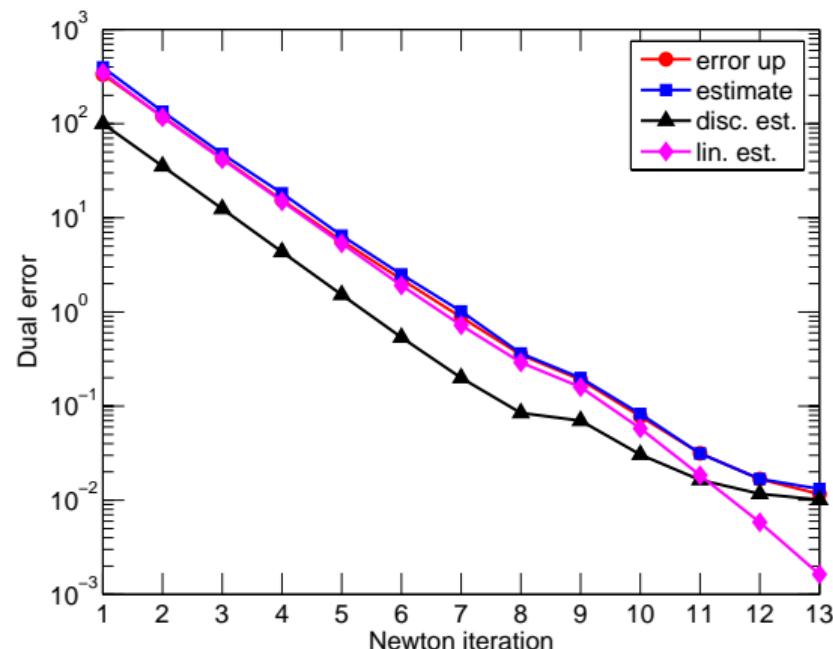
adaptive inexact Newton

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

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



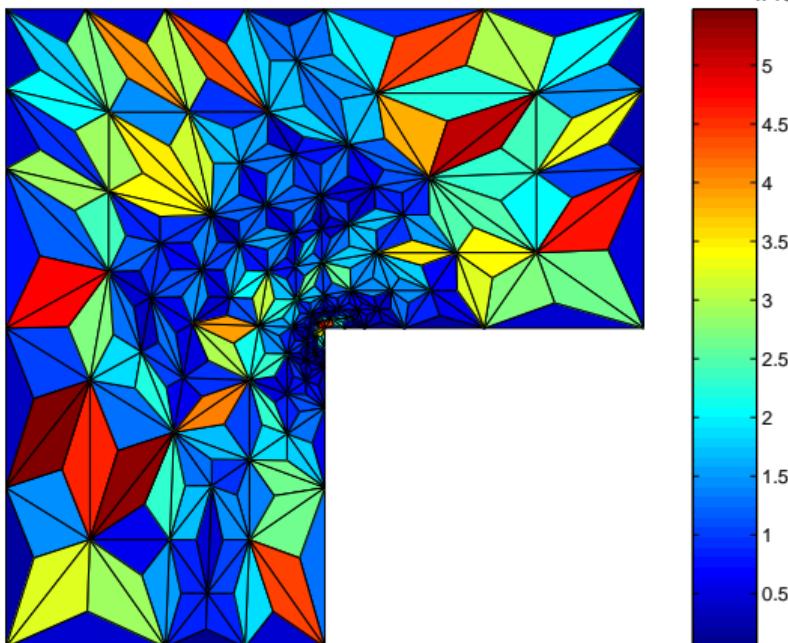
Newton



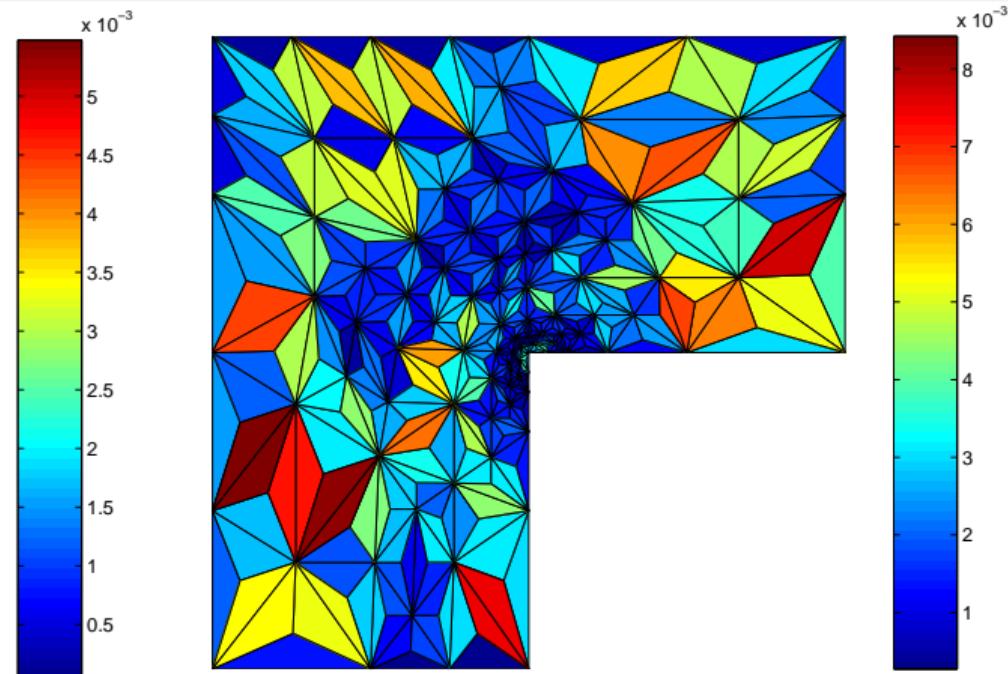
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Nonlinear pb $-\nabla \cdot \sigma(\nabla p) = f$: including **linearization** and **algebraic error**: $\mathcal{U}_\ell(\mathbf{P}_\ell^{k,i}) \neq \mathbf{F}_\ell$, $\mathbb{U}_\ell^{k-1} \mathbf{P}_\ell^{k,i} \neq \mathbf{F}_\ell^{k-1}$

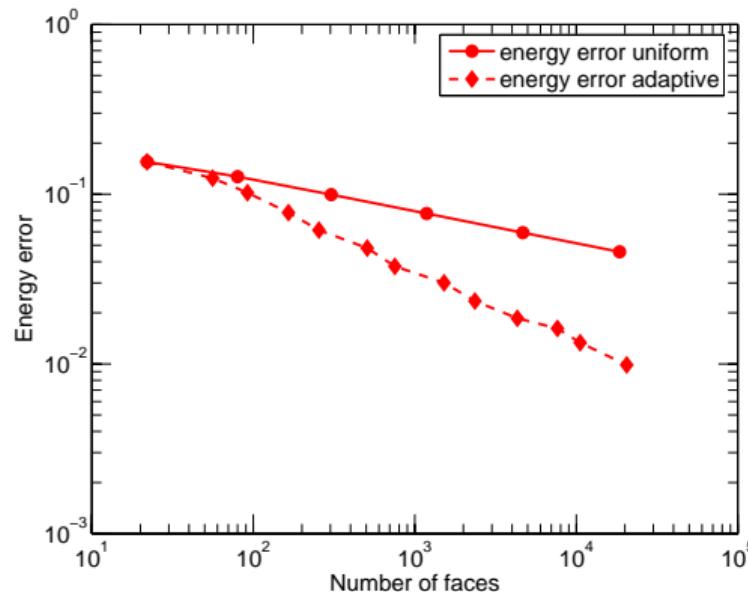


Estimated errors $\eta_K(p_\ell^{k,i})$



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

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

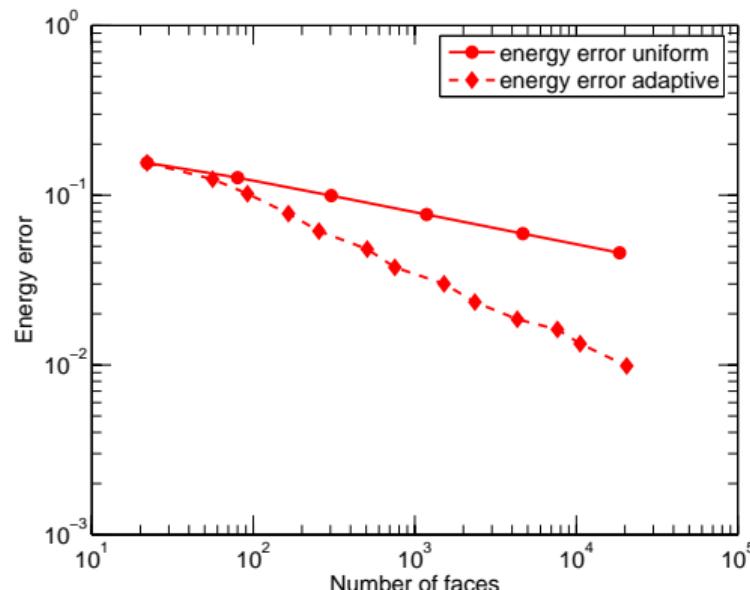
classical

| | |
|------------------------------|-------|
| total alg. solver iterations | 10890 |
| relative error estimate | 4.6% |

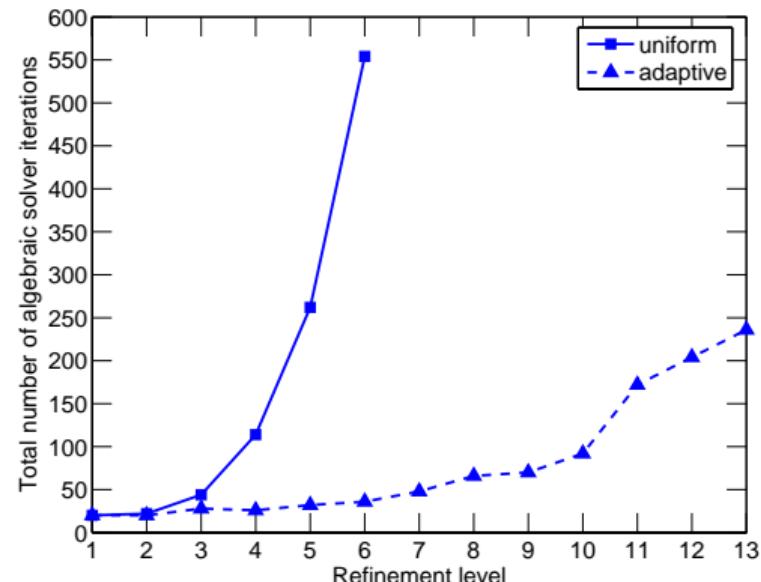
adaptive

| | |
|------------------------------|------|
| total alg. solver iterations | 242 |
| relative error estimate | 1.1% |

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

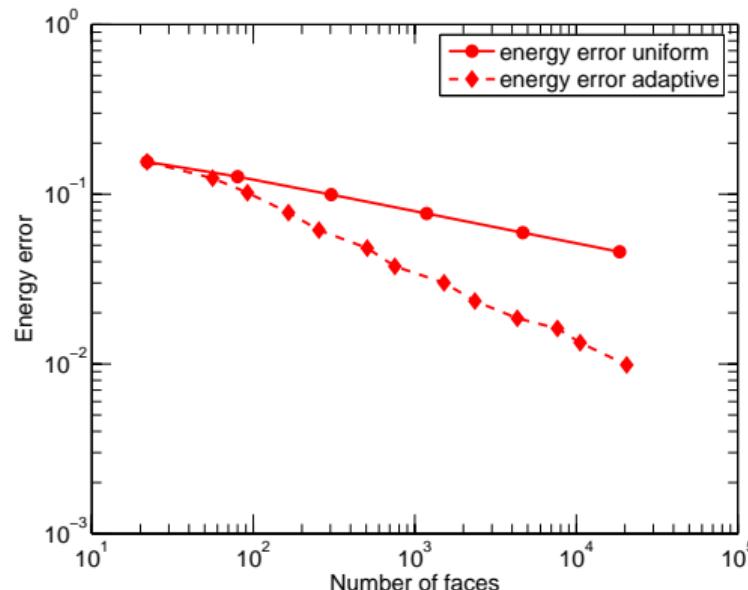


Optimal computational cost

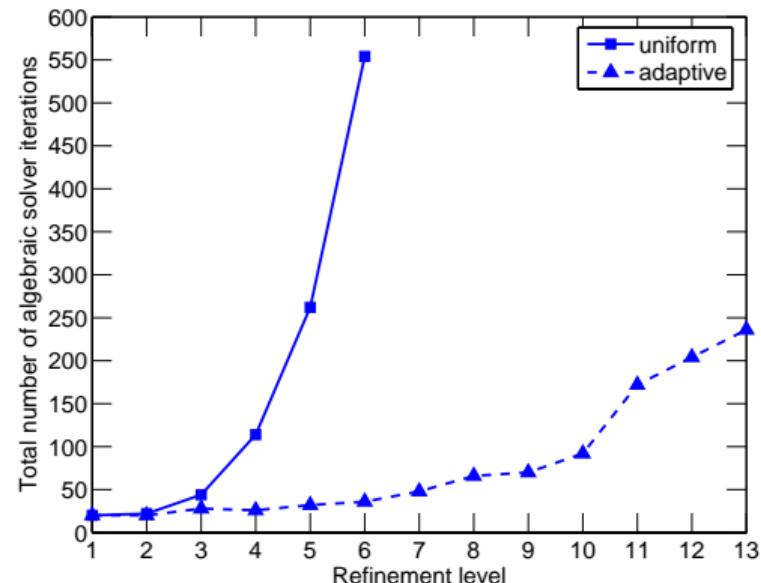
| | | |
|-----------|------------------------------|-------|
| classical | total alg. solver iterations | 10890 |
| | relative error estimate | 4.6% |

| | | |
|----------|------------------------------|------|
| adaptive | total alg. solver iterations | 242 |
| | relative error estimate | 1.1% |

Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs

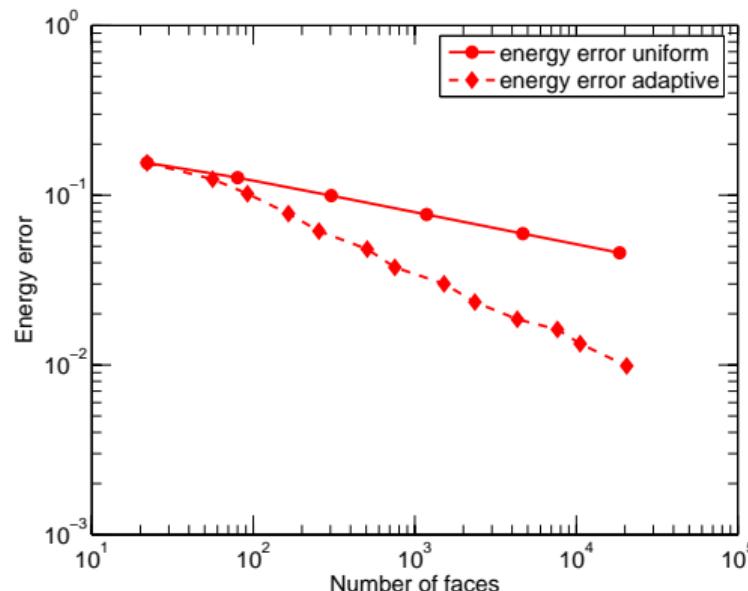


Optimal computational cost

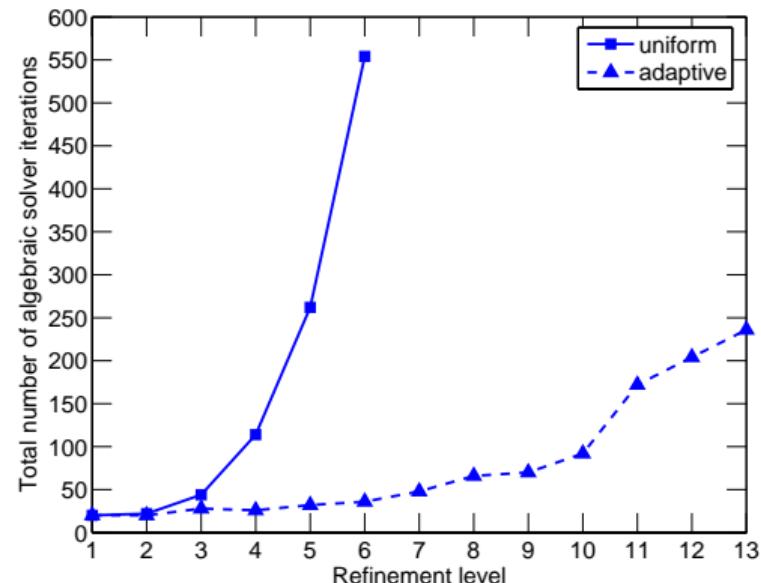
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Convergence and optimal decay rate wrt DoFs & computational cost



Optimal decay rate wrt DoFs



Optimal computational cost

| | | |
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| | | |
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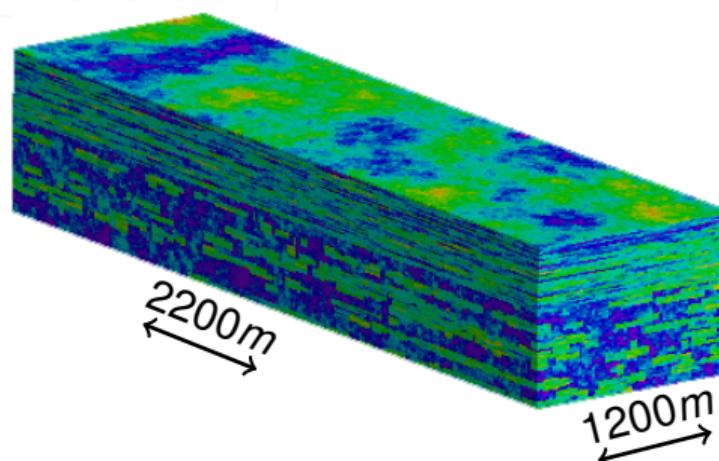
Outline

- 1 Introduction: context, motivation, and goals
- 2 Steady linear Darcy flow
 - Discretization
 - A posteriori error estimate
 - Numerical experiments
- 3 Adaptivity: mesh, polynomial degree, linear solvers, nonlinear solvers
 - Mesh and polynomial degree
 - Linear and nonlinear solvers
 - **Error in a quantity of interest**
- 4 Unsteady multi-phase multi-compositional Darcy flow
- 5 Conclusions

Can we certify error in a practical case $-\nabla \cdot (\mathbf{K} \nabla p) = f$: outflow error

Second step: **goal functional**

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



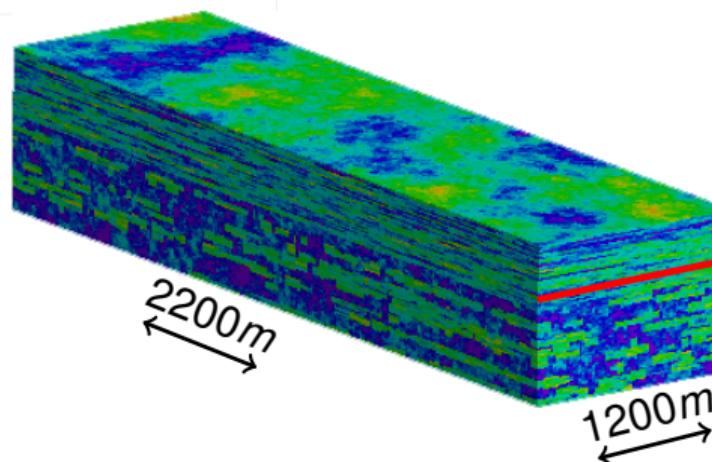
Underground reservoir,
10th SPE test case

© Institut für Geometrie und Praktische Mathematik, Aachen University, 2013-2014

Can we certify error in a practical case $-\nabla \cdot (\mathbf{K} \nabla p) = f$: outflow error

$$\left| \int_{y=2200} \mathbf{K} \nabla(p - p_\ell) \cdot \mathbf{n} \right| \text{ (goal functional)}$$

| | | | |
|-----------------|-----|------|-------|
| no of unknowns | 825 | 3300 | 13200 |
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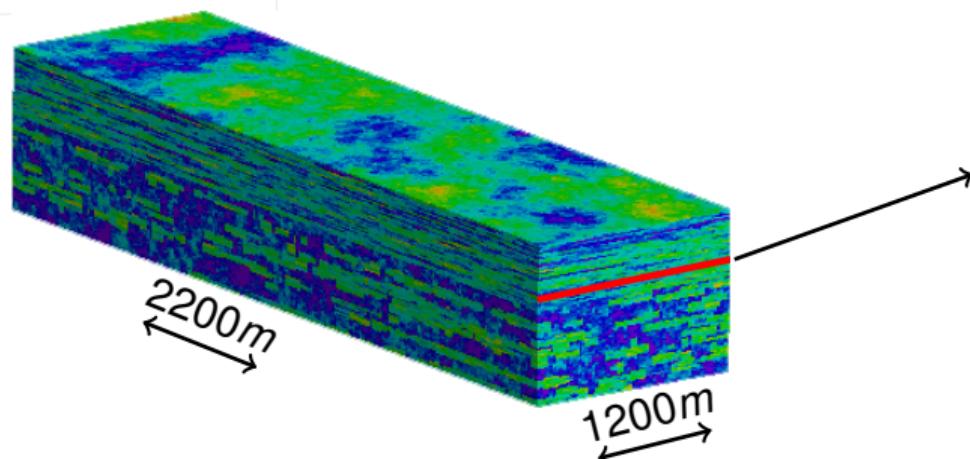
Underground reservoir,
10th SPE test case

G. Mekkaoui, M. Vohralík, Journal of Computational and Applied Mathematics (2019)

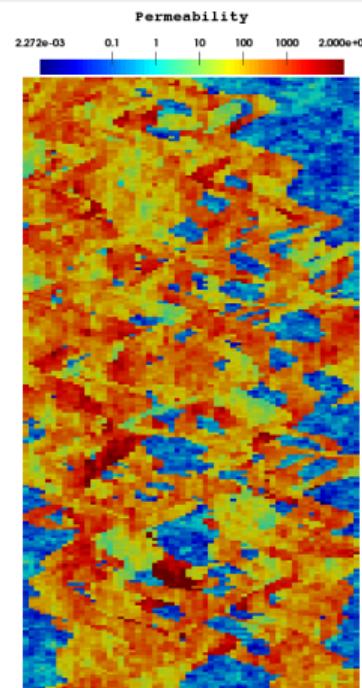
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$|\int_{y=2200} \mathbf{K} \nabla(p - p_\ell) \cdot \mathbf{n}|$ (goal functional)

| | | | |
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Underground reservoir,
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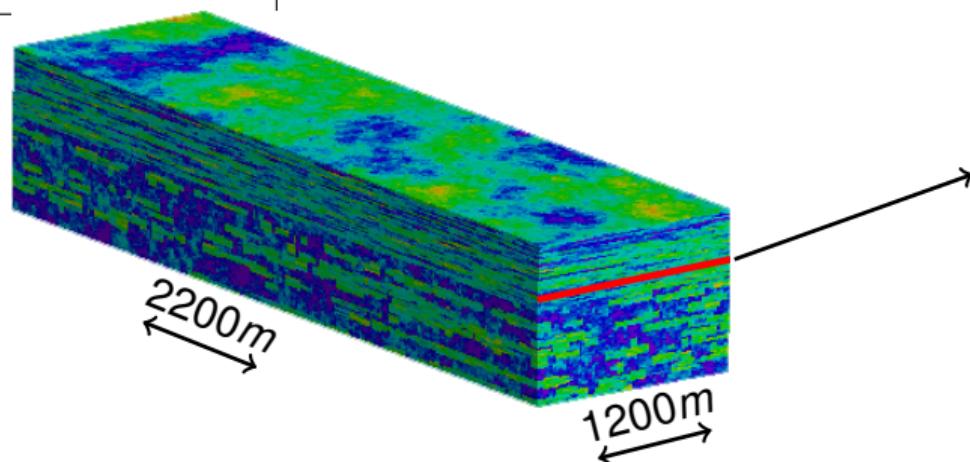
Layer permeability

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

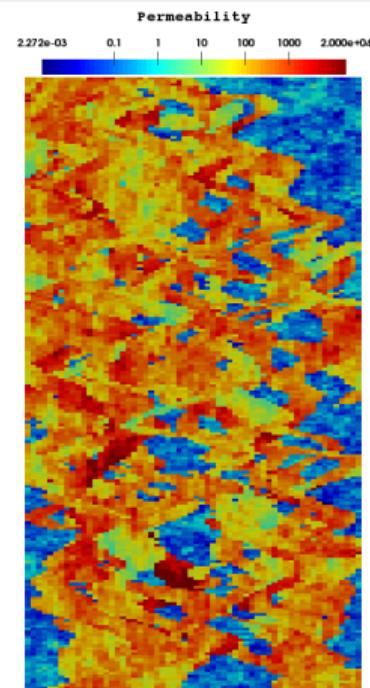
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| | | | |
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Two-phase flow

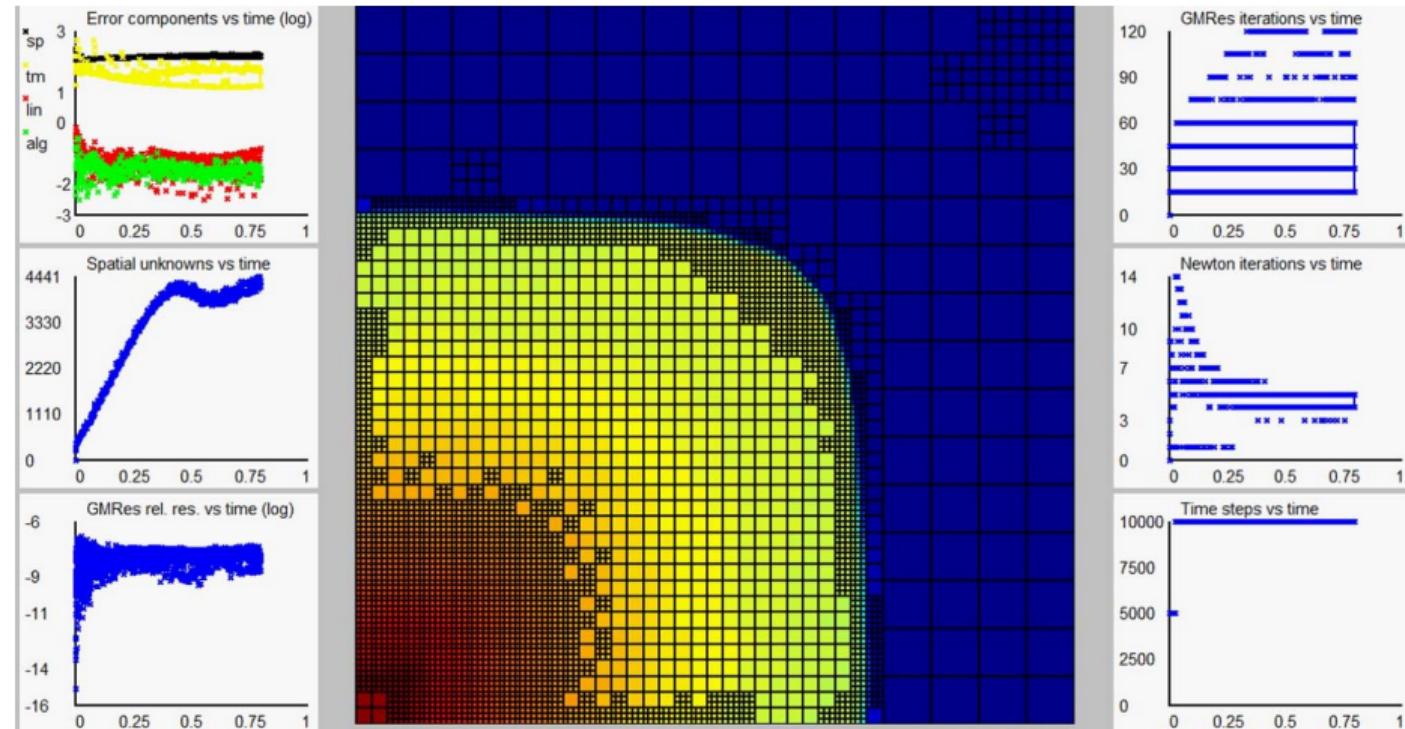
Incompressible two-phase flow in porous media

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

$$\begin{aligned} \partial_t(\phi s_\alpha) - \nabla \cdot \left(\frac{k_{r,\alpha}(s_w)}{\mu_\alpha} \mathbf{K} (\nabla p_\alpha + \rho_\alpha g \nabla z) \right) &= q_\alpha, \quad \alpha \in \{g, w\}, \\ s_g + s_w &= 1, \\ p_g - p_w &= p_c(s_w) \end{aligned}$$

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

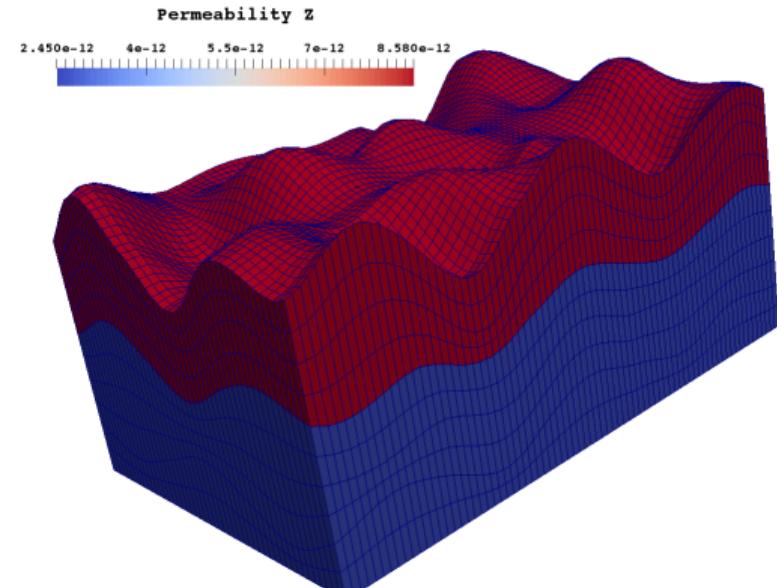
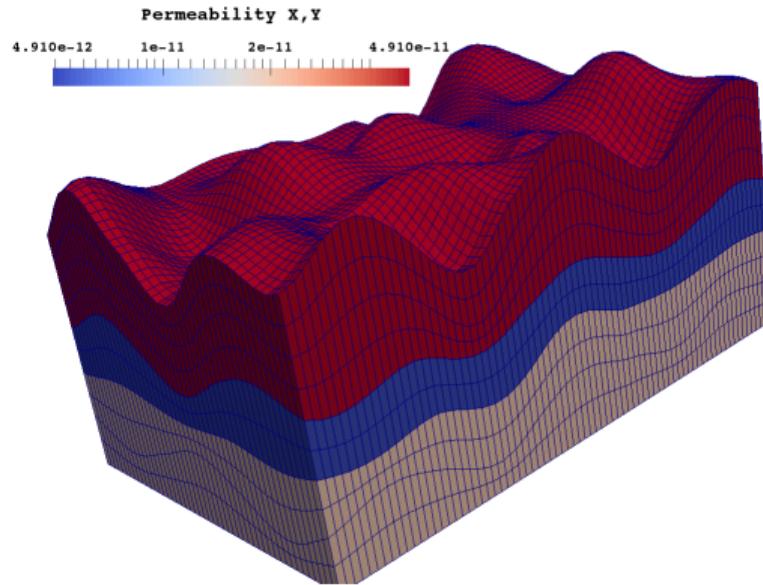
Space/time/nonlinear solver/linear solver adaptivity



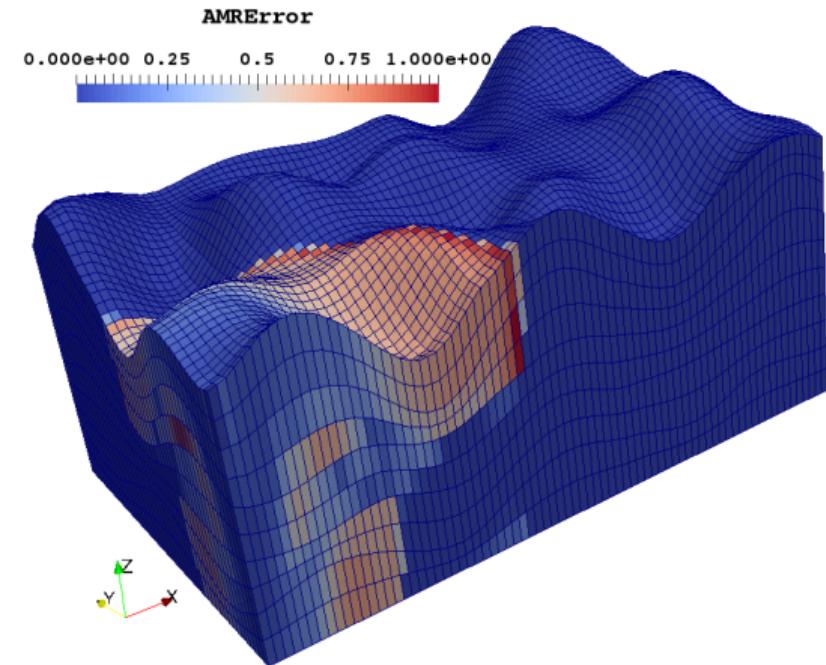
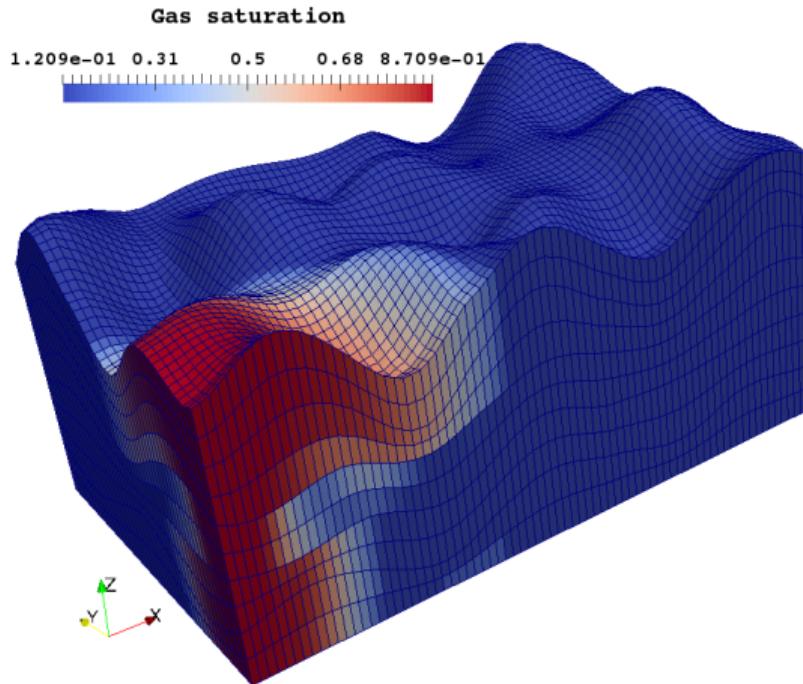
Fully adaptive computation

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

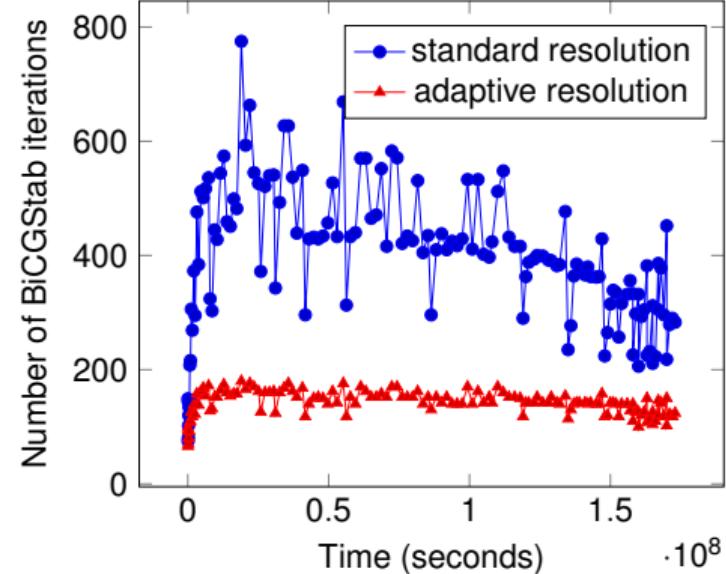
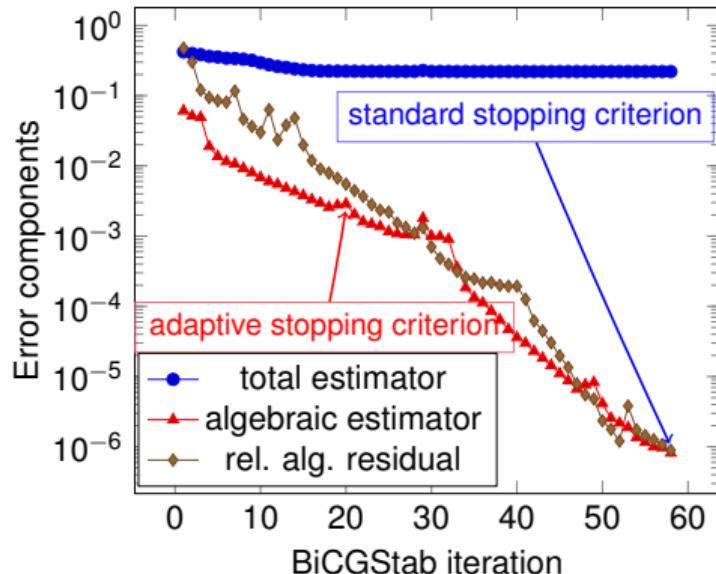
3 phases, 3 components (black-oil) problem: permeability



3 phases, 3 components (black-oil) problem: gas saturation and a posteriori estimate

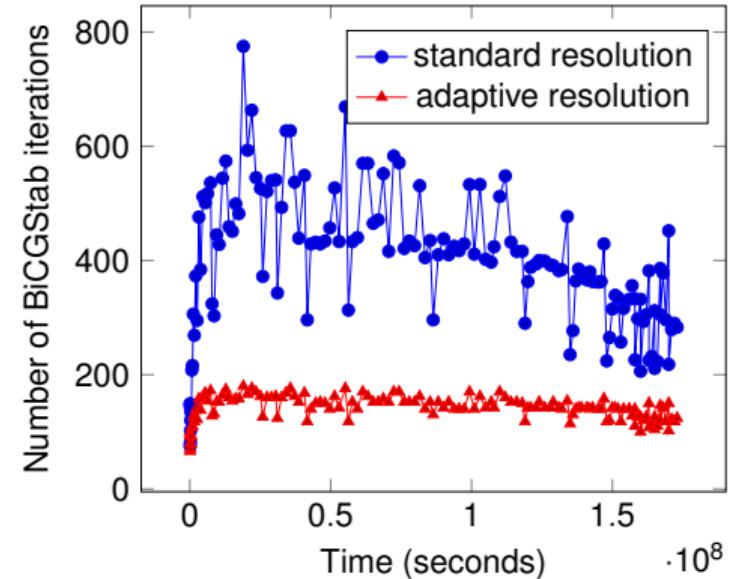
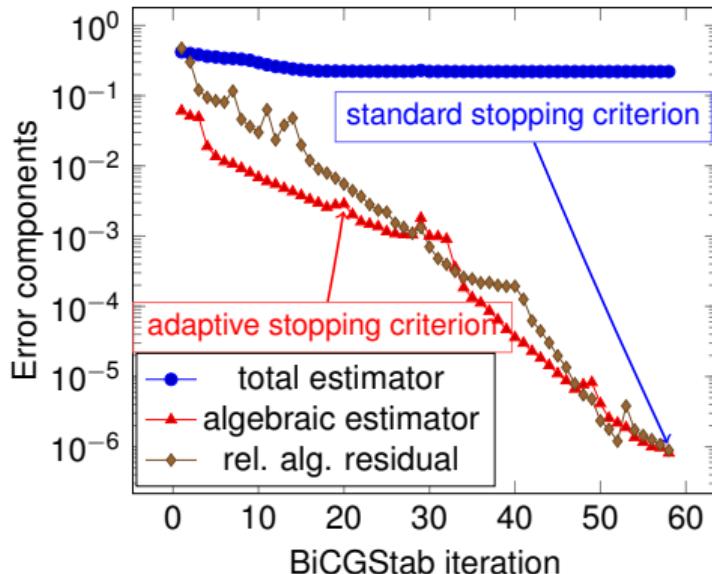


3 phases, 3 components (black-oil): alg. solver & mesh adaptivity



| | Linear solver steps | Resolution time | AMR time | Estimators evaluation | Gain factor |
|---------------------|---------------------|-----------------|----------|-----------------------|-------------|
| Standard resolution | 66386 | 1023s | - | - | - |
| Adaptive resolution | 20184 | 201s | 42s | 26s | 3.8 |

3 phases, 3 components (black-oil): alg. solver & mesh adaptivity



| | Linear solver steps | Resolution time | AMR time | Estimators evaluation | Gain factor |
|---------------------|---------------------|-----------------|----------|-----------------------|-------------|
| Standard resolution | 66386 | 1023s | - | - | - |
| Adaptive resolution | 20184 | 201s | 42s | 26s | 3.8 |

Outline

- 1 Introduction: context, motivation, and goals
- 2 Steady linear Darcy flow
 - Discretization
 - A posteriori error estimate
 - Numerical experiments
- 3 Adaptivity: mesh, polynomial degree, linear solvers, nonlinear solvers
 - Mesh and polynomial degree
 - Linear and nonlinear solvers
 - Error in a quantity of interest
- 4 Unsteady multi-phase multi-compositional Darcy flow
- 5 Conclusions

Conclusions

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- **full adaptivity**: linear solver, nonlinear solver, time step, space mesh (*hp*)
- intrinsically leads to **mass balance recovery** in any situation

Ongoing work

- convergence and optimality proofs
- application to challenging porous media problems

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