

# Contrôle d'erreur numérique a posteriori et critères d'arrêt pour des solveurs linéaires et non linéaires

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Méthodes récentes pour la résolution  
de systèmes linéaires et non linéaires  
dans le contexte du calcul haute performance,  
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# Outline

## 1 Introduction

## 2 Adaptive inexact Newton method

- A guaranteed a posteriori error estimate
- Stopping criteria and efficiency
- Applications
- Numerical results

## 3 Application to two-phase flow in porous media

- A guaranteed a posteriori error estimate
- Application and numerical results

## 4 Conclusions and future directions

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# Inexact Newton method

## 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 linearization)

1 Choose initial vector  $U^0$ . Set  $k := 1$ .

2  $U^{k-1} \Rightarrow$  matrix  $\mathbb{A}^{k-1}$  and vector  $F^{k-1}$ : find  $U^k$  s.t.

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

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# Context and questions

## Approximate solution

- approximate solution  $U^{k,i}$  does **not solve**  $\mathcal{A}(U^{k,i}) = F$

## Numerical method

- underlying numerical method: the vector  $U^{k,i}$  is associated with a (piecewise polynomial) **approximation**  $u_h^{k,i}$

## Partial differential equation

- underlying PDE,  $u$  its **weak solution**:  $A(u) = f$

### Question (Stopping criteria)

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

### Question (Error)

- *How big is the error  $\|u - u_h^{k,i}\|$  on Newton step  $k$  and algebraic solver step  $i$ , how is it distributed?*

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# Previous results

## Inexact Newton method

- Eisenstat and Walker (1990's) (conception, convergence, a priori error estimates)
- Moret (1989) (discrete a posteriori error estimates)

## Adaptive inexact Newton method

- Bank and Rose (1982), combination with multigrid
- Hackbusch and Reusken (1989), damping and multigrid
- Deuflhard (1990's, 2004 book), adaptive damping and multigrid

## Stopping criteria for algebraic solvers

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

## A posteriori error estimates for numerical discretizations of nonlinear problems

- Ladevèze (since 1990's), guaranteed upper bound
- Han (1994), general framework
- Verfürth (1994), residual estimates
- Carstensen and Klose (2003), guaranteed estimates
- Chaillou and Suri (2006, 2007), distinguishing discretization and linearization errors
- Kim (2007), guaranteed estimates, locally conservative methods

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# Quasi-linear elliptic problem

## Quasi-linear elliptic problem

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

- quasi-linear diffusion problem

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

- Leray–Lions problem

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

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

### Example

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

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

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

### Weak formulation

Find  $u \in V$  such that

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# Approximate solution and error measure

## Approximate solution

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

## Error measure

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

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

- weak difference of the fluxes (dual norm of the residual) + nonconformity (computable jump term)
- there holds  $\mathcal{J}_u(u_h^{k,i}) = 0$  if and only if  $u = u_h^{k,i}$
- physical relevance: strong difference of the fluxes + nonconformity

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


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

- weak difference of the fluxes (dual norm of the residual) + nonconformity (computable jump term)
- there holds  $\mathcal{J}_u(u_h^{k,i}) = 0$  if and only if  $u = u_h^{k,i}$
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# Approximate solution and error measure

## Approximate solution

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

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- A guaranteed a posteriori error estimate
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# A posteriori error estimate

## Assumption A (Total flux reconstruction)

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

$$\nabla \cdot \mathbf{t}_h^{k,i} = f_h - \rho_h^{k,i},$$

*with the data approximation  $f_h$  s.t.  $(f_h, 1)_K = (f, 1)_K \quad \forall K \in \mathcal{T}_h$ .*

## Theorem (A guaranteed a posteriori error estimate)

Let

- $u \in V$  be the weak solution,
- $u_h^{k,i} \in V(\mathcal{T}_h)$  be arbitrary,
- Assumption A hold.

Then there holds

$$\mathcal{J}_u(u_h^{k,i}) \leq \bar{\eta}^{k,i},$$

where  $\bar{\eta}^{k,i}$  is fully computable from  $u_h^{k,i}$ ,  $\mathbf{t}_h^{k,i}$ , and  $\rho_h^{k,i}$ .

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# Distinguishing error components

Assumption B (Discretization, linearization, and algebraic errors)

There exist fluxes  $\mathbf{d}_h^{k,i}, \mathbf{l}_h^{k,i}, \mathbf{a}_h^{k,i} \in [L^q(\Omega)]^d$  such that

- (i)  $\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i} + \mathbf{a}_h^{k,i} = \mathbf{t}_h^{k,i};$
- (ii) as the linear solver converges,  $\|\mathbf{a}_h^{k,i}\|_q \rightarrow 0;$
- (iii) as the nonlinear solver converges,  $\|\mathbf{l}_h^{k,i}\|_q \rightarrow 0.$

## Comments

- $\mathbf{d}_h^{k,i}$ : *discretization flux reconstruction*
- $\mathbf{l}_h^{k,i}$ : *linearization error flux reconstruction*
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# Estimate distinguishing error components

## Theorem (Estimate distinguishing different error components)

Let

- $u \in V$  be the weak solution,
- $u_h^{k,i} \in V(\mathcal{T}_h)$  be arbitrary,
- Assumptions A and B hold.

Then there holds

$$\mathcal{J}_u(u_h^{k,i}) \leq \eta^{k,i} := \eta_{\text{disc}}^{k,i} + \eta_{\text{lin}}^{k,i} + \eta_{\text{alg}}^{k,i} + \eta_{\text{rem}}^{k,i} + \eta_{\text{quad}}^{k,i} + \eta_{\text{osc}}^{k,i}.$$

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# Estimators

- *discretization* estimator

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

- *linearization* estimator

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

- *algebraic* estimator

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

- *algebraic remainder estimator*

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

- *quadrature estimator*

$$\eta_{\text{quad},K}^{k,i} := \|\boldsymbol{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}) - \bar{\sigma}_h^{k,i}\|_{q,K}$$

- *data oscillation estimator*

$$\eta_{\text{osc},K}^{k,i} := C_{\text{P},p} h_K \|f - f_h\|_{q,K}$$

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

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# Stopping criteria

## Global stopping criteria

- stop whenever:

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

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

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

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

## Local stopping criteria

- stop whenever:

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

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

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

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# Assumption for efficiency

## Assumption C (Approximation property)

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

$$\|\bar{\sigma}_h^{k,i} + \mathbf{d}_h^{k,i}\|_{q,K} \lesssim \eta_{\sharp,\mathfrak{T}_K}^{k,i} + \eta_{\text{osc},\mathfrak{T}_K}^{k,i},$$

where

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

# Global efficiency

## Theorem (Global efficiency)

Let the mesh  $T_h$  be shape-regular and let the **global stopping criteria** hold. Recall that  $\mathcal{J}_u(u_h^{k,i}) \leq \eta^{k,i}$ . Then, under Assumption C,

$$\eta^{k,i} \lesssim \mathcal{J}_u(u_h^{k,i}) + \eta_{\text{quad}}^{k,i} + \eta_{\text{osc}}^{k,i},$$

where  $\lesssim$  means up to a constant **independent** of  $\sigma$  and  $q$ .

- **robustness** with respect to the **nonlinearity** thanks to the choice of the **dual norm** as error measure

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

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# Algebraic error flux reconstruction and algebraic remainder

## Construction of $\mathbf{a}_h^{k,i}$ and $\rho_h^{k,i}$

- On linearization step  $k$  and algebraic step  $i$ , we have

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

- Do  $\nu$  additional steps of the algebraic solver, yielding

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

- Construct the function  $\rho_h^{k,i}$  from the algebraic residual vector  $\mathbf{R}^{k,i+\nu}$  (lifting into appropriate discrete space).
- Suppose we can obtain discretization and linearization flux reconstructions  $\mathbf{d}_h^{k,i}, \mathbf{l}_h^{k,i}$  on each algebraic step. Then set

$$\mathbf{a}_h^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}).$$

- $\nu$  chosen adaptively so that  $\eta_{\text{rem},K}^{k,i}$  or  $\eta_{\text{rem}}^{k,i}$  are small enough.
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$$\mathbf{a}_h^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}).$$

- $\nu$  chosen adaptively so that  $\eta_{\text{rem},K}^{k,i}$  or  $\eta_{\text{rem}}^{k,i}$  are small enough.
- Independent of the algebraic solver.

# Algebraic error flux reconstruction and algebraic remainder

## Construction of $\mathbf{a}_h^{k,i}$ and $\rho_h^{k,i}$

- On linearization step  $k$  and algebraic step  $i$ , we have

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

- Do  $\nu$  additional steps of the algebraic solver, yielding

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# Nonconforming finite elements for the $p$ -Laplacian

## Discretization

Find  $\textcolor{orange}{u}_h \in V_h$  such that

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

- $\sigma(\nabla u_h) = |\nabla u_h|^{p-2} \nabla u_h$
- $V_h$  the Crouzeix–Raviart space
- $f_h := \Pi_0 f$
- leads to the system of **nonlinear algebraic equations**

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

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# Linearization

## Linearization

Find  $\textcolor{brown}{u}_h^k \in V_h$  such that

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

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

- Newton linearization

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

- leads to the system of linear algebraic equations

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## Algebraic solution

Find  $\textcolor{red}{u}_h^{k,i} \in V_h$  such that

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- algebraic residual vector  $R^{k,i} = \{R_e^{k,i}\}_{e \in \mathcal{E}_h^{\text{int}}}$
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# Flux reconstructions

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

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

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

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Set  $\bar{\sigma}_h^{k,i} := \sigma(\nabla u_h^{k,i})$ . Consequently,  $\eta_{\text{quad}, K}^{k,i} = 0$  for all  $K \in \mathcal{T}_h$ .

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# Verification of the assumptions – upper bound

## Lemma (Assumptions A and B)

*Assumptions A and B hold.*

## Comments

- $\|\mathbf{a}_h^{k,i}\|_{q,K} \rightarrow 0$  as the linear solver converges by definition.
- $\|\mathbf{l}_h^{k,i}\|_{q,K} \rightarrow 0$  as the nonlinear solver converges by the construction of  $\mathbf{l}_h^{k,i}$ .
- Both  $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i})$  and  $\mathbf{d}_h^{k,i}$  belong to  $\mathbf{RTN}_0(\mathcal{S}_h) \Rightarrow \mathbf{a}_h^{k,i} \in \mathbf{RTN}_0(\mathcal{S}_h)$  and  $\mathbf{t}_h^{k,i} \in \mathbf{RTN}_0(\mathcal{S}_h)$ .

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# Verification of the assumptions – efficiency

## Lemma (Assumption C)

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- $\mathbf{d}_h^{k,i}$  close to  $\sigma(\nabla u_h^{k,i})$
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# Discontinuous Galerkin for the quasi-linear diffusion

## Discretization

Find  $\textcolor{red}{u}_h \in V_h := \mathbb{P}_m(\mathcal{T}_h)$ ,  $m \geq 1$ , such that, for all  $v_h \in V_h$ ,

$$\begin{aligned} & (\sigma(u_h, \nabla u_h), \nabla v_h) - \sum_{e \in \mathcal{E}_h} \left\{ \langle \{\!\{ \sigma(u_h, \nabla u_h) \}\!\} \cdot \mathbf{n}_e, [\![ v_h ]\!] \rangle_e \right. \\ & \left. + \theta \langle \{\!\{ \underline{\mathbf{A}}(u_h) \nabla v_h \}\!\} \cdot \mathbf{n}_e, [\![ u_h ]\!] \rangle_e \right\} + \sum_{e \in \mathcal{E}_h} \langle \bar{\alpha}_e h_e^{-1} [\![ u_h ]\!], [\![ v_h ]\!] \rangle_e = (f, v_h). \end{aligned}$$

- $\theta \in \{-1, 0, 1\}$
- $\bar{\alpha}_e := \|\underline{\mathbf{A}}\|_{L^\infty(\mathbb{R})} \chi_e$ ,  $\chi_e$  large enough
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- algebraic residual vector  $R^{k,i} = \{R_{K,j}^{k,i}\}_{K \in \mathcal{T}_h, j \in \mathcal{C}_K}$
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# Flux reconstructions

Definition (Construction of  $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \in \mathbf{RTN}_l(\mathcal{T}_h)$ ,  $l := m-1|m$ )

For all  $K \in \mathcal{T}_h$  and all  $e \in \mathcal{E}_K$ ,

$$\langle (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \cdot \mathbf{n}_e, q_h \rangle_e := \langle -\{\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i})\} \cdot \mathbf{n}_e + \bar{\alpha}_e h_e^{-1} \llbracket u_h^{k,i} \rrbracket, q_h \rangle_e,$$

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for all  $q_h \in \mathbb{P}_l(e)$  and all  $\mathbf{r}_h \in [\mathbb{P}_{l-1}(K)]^d$ .

Definition (Construction of  $\mathbf{d}_h^{k,i} \in \mathbf{RTN}_l(\mathcal{T}_h)$ ,  $l := m-1$  or  $l := m$ )

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# Flux reconstructions

Definition (Construction of  $(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \in \mathbf{RTN}_l(\mathcal{T}_h)$ ,  $l := m-1|m$ )

For all  $K \in \mathcal{T}_h$  and all  $e \in \mathcal{E}_K$ ,

$$\langle (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}) \cdot \mathbf{n}_e, q_h \rangle_e := \langle -\{\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i})\} \cdot \mathbf{n}_e + \bar{\alpha}_e h_e^{-1} \llbracket u_h^{k,i} \rrbracket, q_h \rangle_e,$$

$$(\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i}, \mathbf{r}_h)_K := -(\sigma^{k-1}(u_h^{k,i}, \nabla u_h^{k,i}), \mathbf{r}_h)_K$$

$$+ \theta \sum_{e \in \mathcal{E}_K} w_e \langle \mathbf{A}^{k-1}(u_h^{k,i}) \mathbf{r}_h \cdot \mathbf{n}_e, \llbracket u_h^{k,i} \rrbracket \rangle_e,$$

for all  $q_h \in \mathbb{P}_l(e)$  and all  $\mathbf{r}_h \in [\mathbb{P}_{l-1}(K)]^d$ .

Definition (Construction of  $\mathbf{d}_h^{k,i} \in \mathbf{RTN}_l(\mathcal{T}_h)$ ,  $l := m-1$  or  $l := m$ )

For all  $K \in \mathcal{T}_h$  and all  $e \in \mathcal{E}_K$ ,

$$\langle \mathbf{d}_h^{k,i} \cdot \mathbf{n}_e, q_h \rangle_e := \langle -\{\sigma(u_h^{k,i}, \nabla u_h^{k,i})\} \cdot \mathbf{n}_e + \bar{\alpha}_e h_e^{-1} \llbracket u_h^{k,i} \rrbracket, q_h \rangle_e,$$

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for all  $q_h \in \mathbb{P}_l(e)$  and all  $\mathbf{r}_h \in [\mathbb{P}_{l-1}(K)]^d$ .

# Verification of the assumptions – upper bound

Definition (Construction of  $f_h$ ,  $\bar{\sigma}_h^{k,i}$ )

Set  $f_h := \Pi_I f$  and  $\bar{\sigma}_h^{k,i} := \mathbf{I}_I^{\text{RTN}}(\sigma(u_h^{k,i}, \nabla u_h^{k,i}))$ .

Lemma (Assumptions A and B)

*Assumptions A and B hold.*

## Comments

- $\|\mathbf{a}_h^{k,i}\|_{q,K} \rightarrow 0$  as the linear solver converges by definition.
- $\|\mathbf{I}_h^{k,i}\|_{q,K} \rightarrow 0$  as the nonlinear solver converges by the construction of  $\mathbf{I}_h^{k,i}$ .
- Both  $(\mathbf{d}_h^{k,i} + \mathbf{I}_h^{k,i})$  and  $\mathbf{d}_h^{k,i}$  belong to  $\mathbf{RTN}_I(\mathcal{T}_h) \Rightarrow \mathbf{a}_h^{k,i} \in \mathbf{RTN}_I(\mathcal{T}_h)$  and  $\mathbf{t}_h^{k,i} \in \mathbf{RTN}_I(\mathcal{T}_h)$ .

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# Verification of the assumptions – efficiency

## Lemma (Assumption C)

*Assumption C holds.*

### Comments

- $\mathbf{d}_h^{k,i}$  close to  $\overline{\sigma}_h^{k,i}$
- approximation properties of Raviart–Thomas–Nédélec spaces

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## Lemma (Assumption C)

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# Summary

## Discretization methods

- conforming finite elements
- nonconforming finite elements
- discontinuous Galerkin
- various finite volumes
- mixed finite elements

## Linearizations

- fixed point
- Newton

## Linear solvers

- independent of the linear solver

... all Assumptions A to C verified

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# Outline

## 1 Introduction

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- Stopping criteria and efficiency
- Applications
- Numerical results

## 3 Application to two-phase flow in porous media

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## 4 Conclusions and future directions

# Numerical experiment I

## Model problem

- $p$ -Laplacian

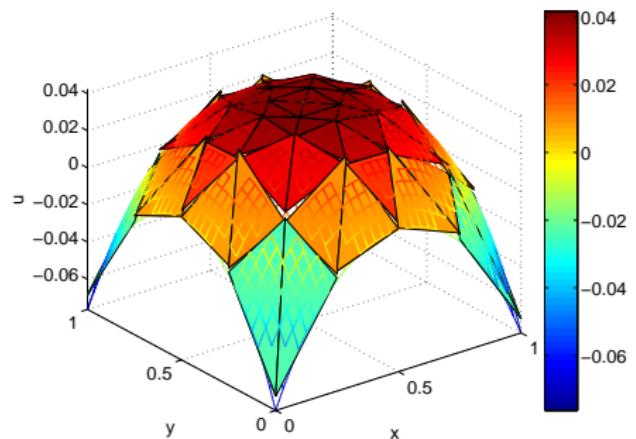
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

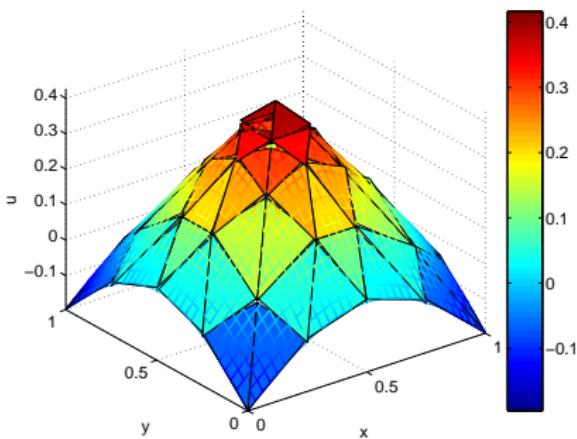
$$u(x, y) = -\frac{p-1}{p} \left( (x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left( \frac{1}{2} \right)^{\frac{p}{p-1}}$$

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

# Analytical and approximate solutions

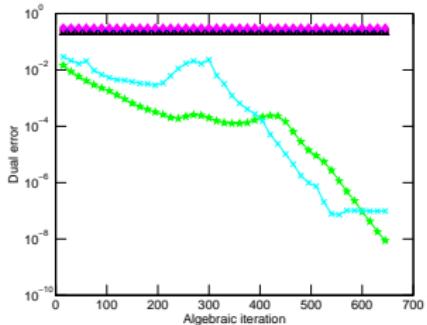


Case  $p = 1.5$

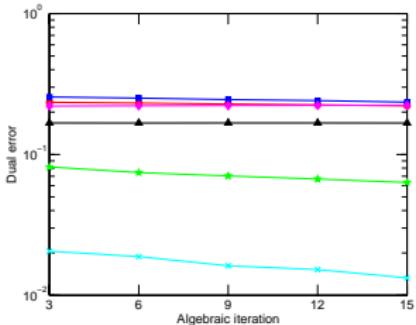


Case  $p = 10$

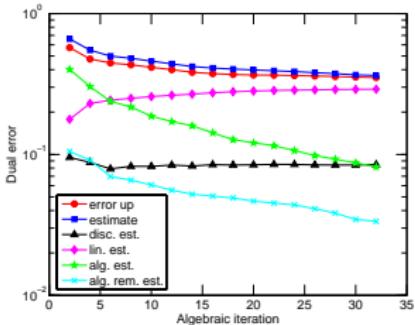
# Error and estimators as a function of CG iterations, $p = 10$ , 6th level mesh, 6th Newton step.



Newton

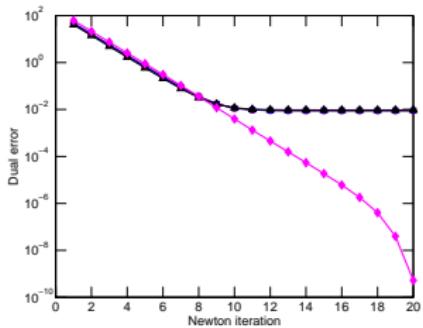


inexact Newton

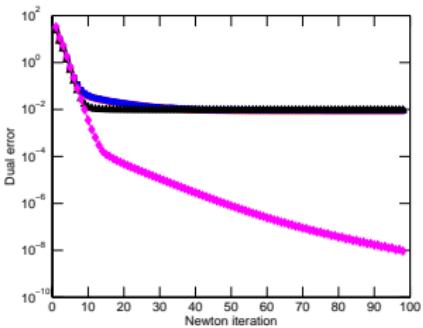


ad. inexact Newton

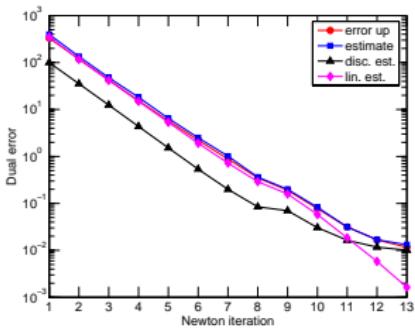
# Error and estimators as a function of Newton iterations, $p = 10$ , 6th level mesh



Newton

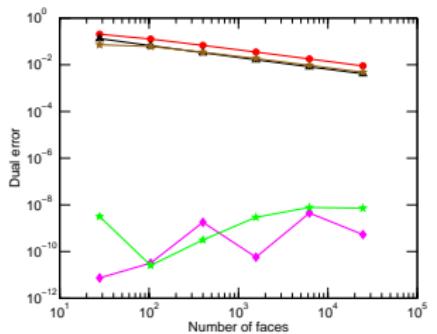


inexact Newton

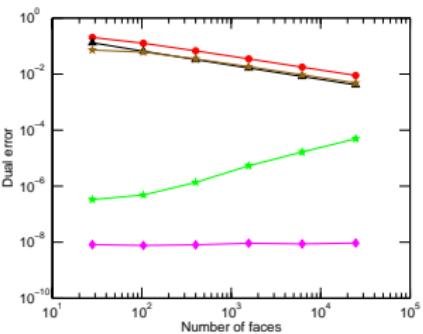


ad. inexact Newton

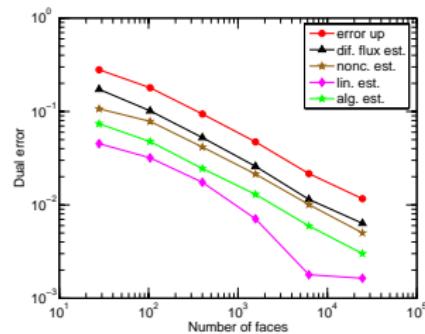
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Newton

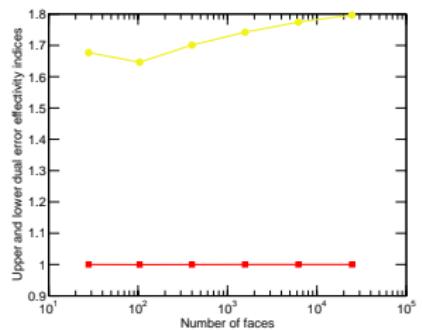


inexact Newton

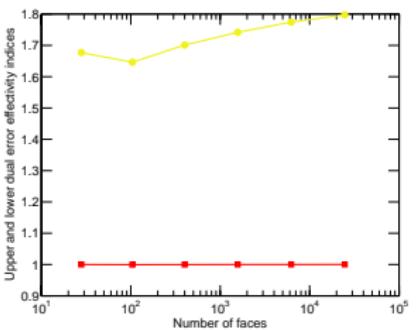


ad. inexact Newton

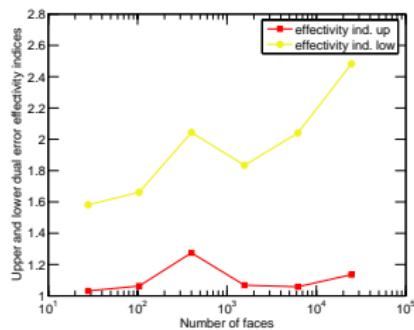
# Effectivity indices, $p = 10$



Newton

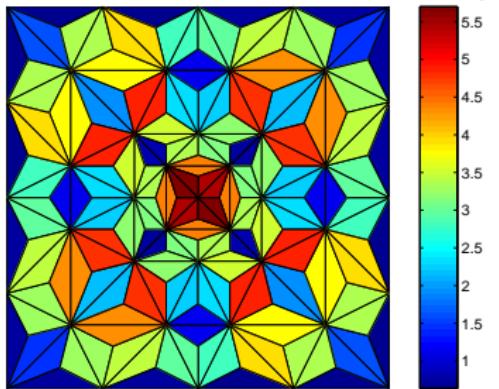


inexact Newton

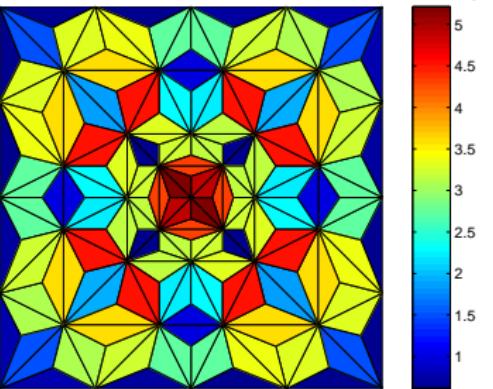


ad. inexact Newton

# Error distribution, $p = 10$

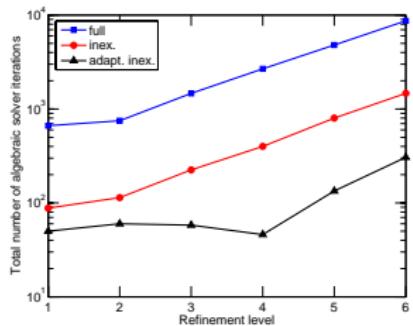
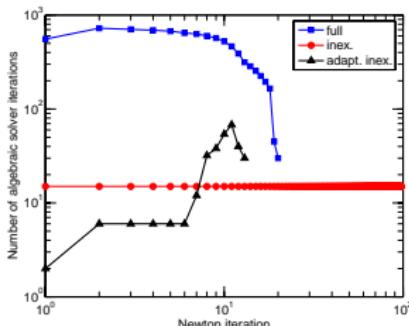
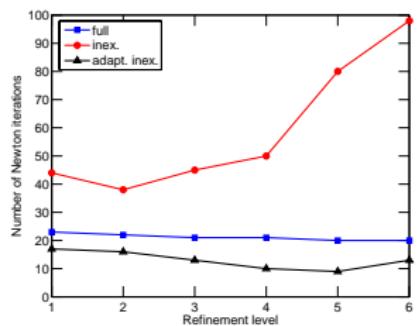


Estimated error distribution



Exact error distribution

# Newton and algebraic iterations, $p = 10$

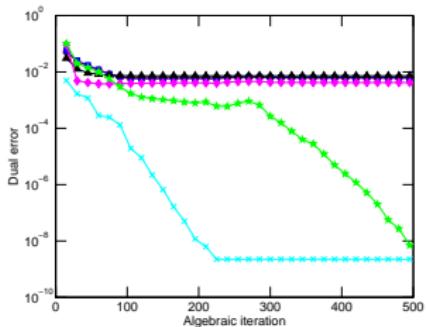


Newton it. / refinement

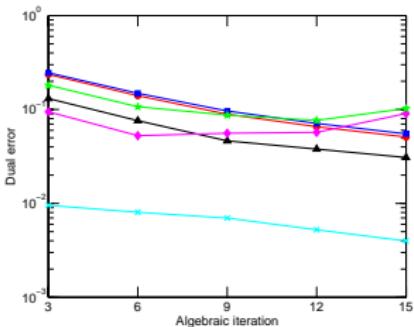
alg. it. / Newton step

alg. it. / refinement

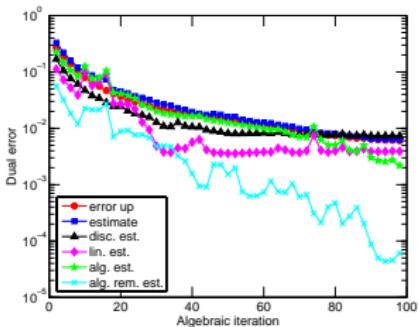
# Error and estimators as a function of CG iterations, $p = 1.5$ , 6th level mesh, 1st Newton step.



Newton

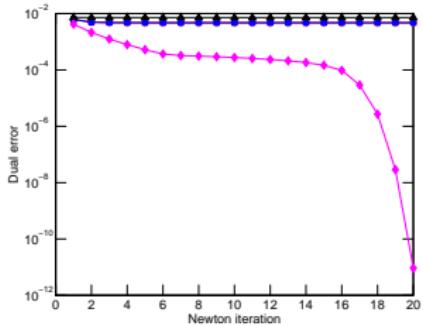


inexact Newton

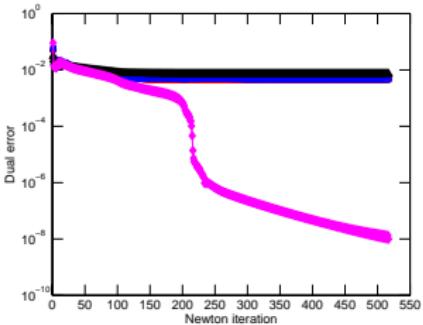


ad. inexact Newton

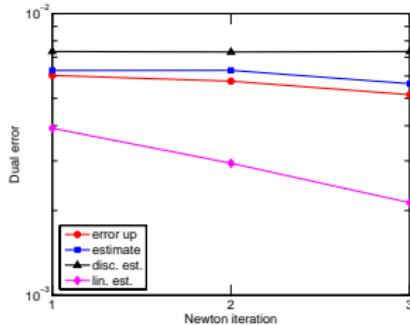
# Error and estimators as a function of Newton iterations, $p = 1.5$ , 6th level mesh



Newton

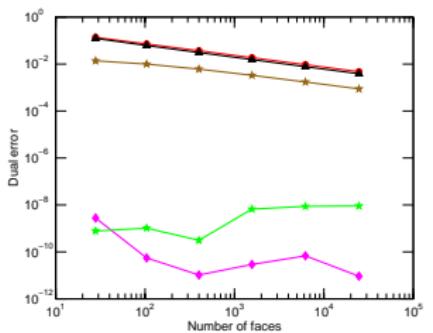


inexact Newton

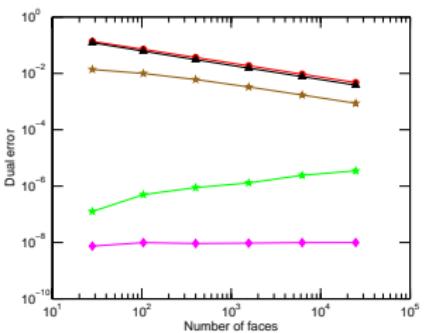


ad. inexact Newton

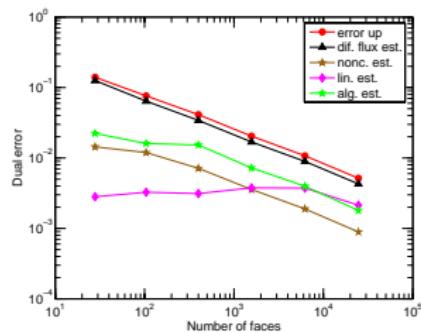
# Error and estimators, $p = 1.5$



Newton

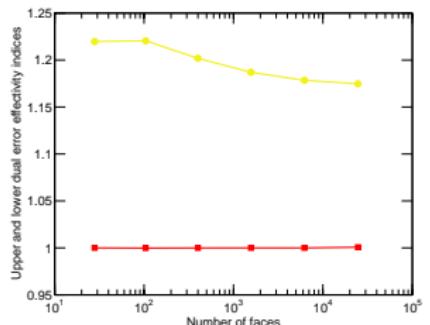


inexact Newton

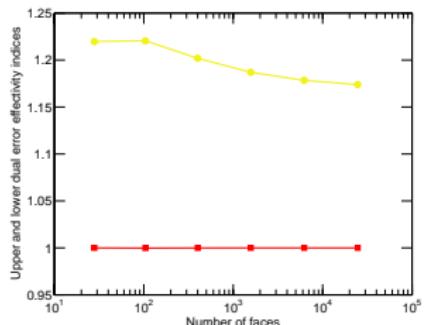


ad. inexact Newton

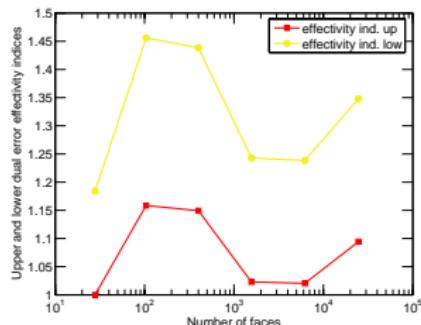
# Effectivity indices, $p = 1.5$



Newton

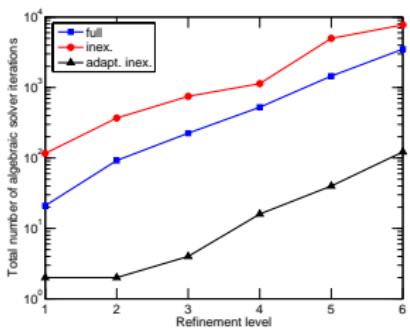
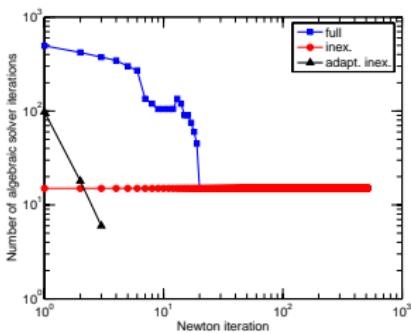
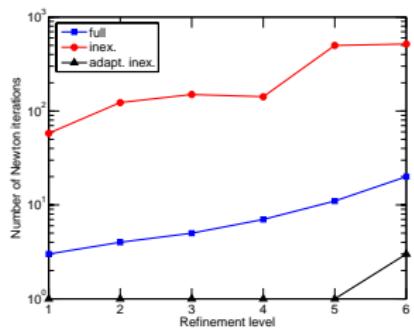


inexact Newton



ad. inexact Newton

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Newton it. / refinement

alg. it. / Newton step

alg. it. / refinement

# Numerical experiment II

## Model problem

- $p$ -Laplacian

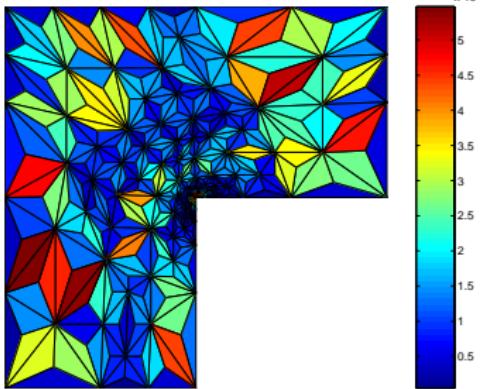
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

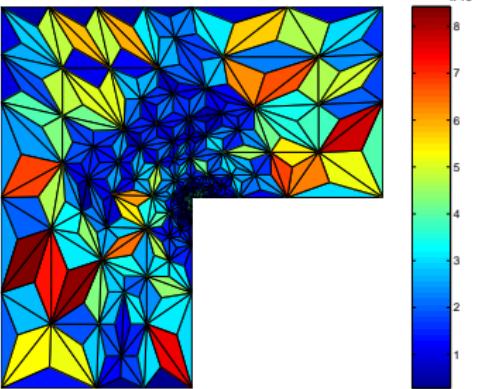
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

# Error distribution on an adaptively refined mesh

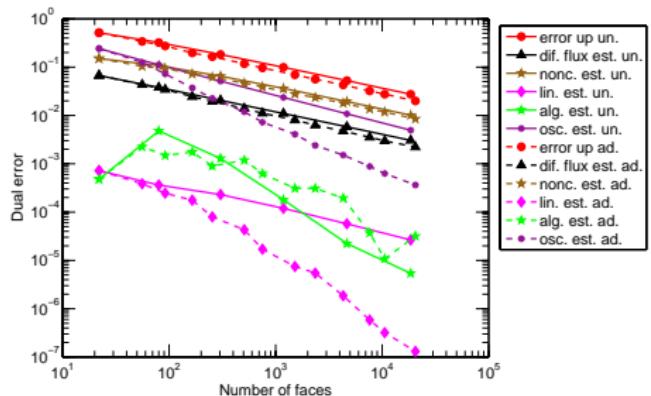


Estimated error distribution

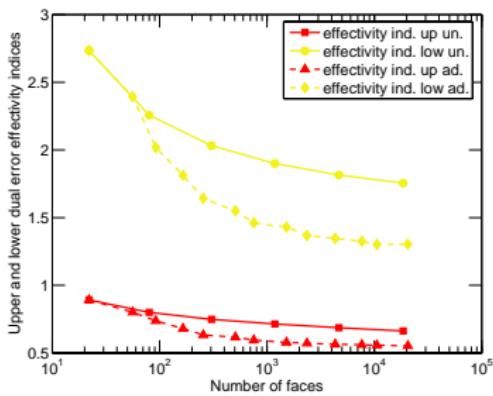


Exact error distribution

# Estimated and actual errors and the effectivity index

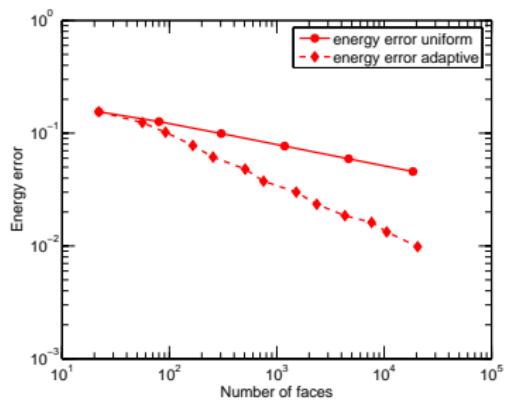


Estimated and actual errors

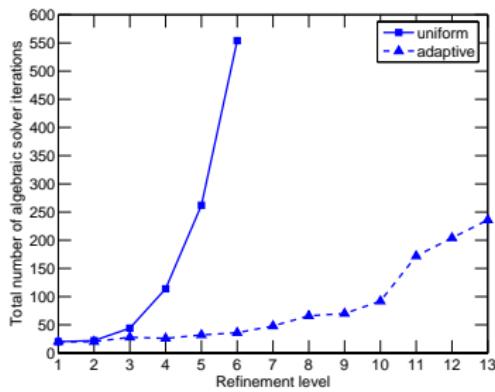


Effectivity index

# Energy error and overall performance



Energy error



Overall performance

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## 4 Conclusions and future directions

# Two-phase flow in porous media

## Two-phase flow in porous media

$$\begin{aligned} \partial_t(\phi s_\alpha) + \nabla \cdot \mathbf{u}_\alpha &= q_\alpha, & \alpha \in \{\text{n}, \text{w}\}, \\ -\lambda_\alpha(s_w) \mathbf{K}(\nabla p_\alpha + \rho_\alpha g \nabla z) &= \mathbf{u}_\alpha, & \alpha \in \{\text{n}, \text{w}\}, \\ s_n + s_w &= 1, \\ p_n - p_w &= p_c(s_w) \end{aligned}$$

## Mathematical issues

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

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# Two-phase flow in porous media

Theorem (A posteriori error estimate distinguishing the error components)

Let

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

with the approximations  $(s_w^{n,k,i}, p_w^{n,k,i})$ . Then

$$\| (s_w - s_w^{n,k,i}, p_w - p_w^{n,k,i}) \|_{I_n} \leq \eta_{\text{sp}}^{n,k,i} + \eta_{\text{tm}}^{n,k,i} + \eta_{\text{lin}}^{n,k,i} + \eta_{\text{alg}}^{n,k,i}.$$

## Error components

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

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- $\eta_{\text{alg}}^{n,k,i}$ : algebraic solver

# Local estimators

- *spatial estimators*

$$\eta_{\text{sp},K}^{n,k,i}(t) := \left\{ \sum_{\alpha \in \{\text{n}, \text{w}\}} (\|\mathbf{d}_{\alpha,h}^{n,k,i} - \mathbf{v}_\alpha(p_{\text{w},h}^{n,k,i}, s_{\text{w},h}^{n,k,i})\|_K + h_K/\pi \|q_\alpha^n - \partial_t^n(\phi s_{\alpha,h\tau}^{n,k,i}) - \nabla \cdot \mathbf{u}_{\alpha,h}^{n,k,i}\|_K)^2 + (\|\mathbf{K}(\lambda_{\text{w}}(s_{\text{w},h\tau}^{n,k,i}) + \lambda_{\text{n}}(s_{\text{w},h\tau}^{n,k,i})) \nabla (\mathbf{p}(p_{\text{w},h\tau}^{n,k,i}, s_{\text{w},h\tau}^{n,k,i}) - \bar{\mathbf{p}}_{h\tau}^{n,k,i})\|_K(t))^2 + (\|\mathbf{K} \nabla (\mathbf{q}(s_{\text{w},h\tau}^{n,k,i}) - \bar{\mathbf{q}}_{h\tau}^{n,k,i})\|_K(t))^2 \right\}^{\frac{1}{2}}$$

- *temporal estimators*

$$\eta_{\text{tm},K,\alpha}^{n,k,i}(t) := \|\mathbf{v}_\alpha(p_{\text{w},h\tau}^{n,k,i}, s_{\text{w},h\tau}^{n,k,i})(\textcolor{red}{t}) - \mathbf{v}_\alpha(p_{\text{w},h\tau}^{n,k,i}, s_{\text{w},h\tau}^{n,k,i})(\textcolor{red}{t^n})\|_K \quad \alpha \in \{\text{n}, \text{w}\}$$

- *linearization estimators*

$$\eta_{\text{lin},K,\alpha}^{n,k,i} := \|\mathbf{l}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\text{n}, \text{w}\}$$

- *algebraic estimators*

$$\eta_{\text{alg},K,\alpha}^{n,k,i} := \|\mathbf{a}_{\alpha,h}^{n,k,i}\|_K \quad \alpha \in \{\text{n}, \text{w}\}$$

# Global estimators

## Global estimators

$$\eta_{\text{sp}}^{n,k,i} := \left\{ 3 \int_{I^n} \sum_{K \in \mathcal{T}_h^n} (\eta_{\text{sp},K}^{n,k,i}(t))^2 dt \right\}^{\frac{1}{2}},$$

$$\eta_{\text{tm}}^{n,k,i} := \left\{ \sum_{\alpha \in \{\text{n}, \text{w}\}} \int_{I^n} \sum_{K \in \mathcal{T}_h^n} (\eta_{\text{tm},K,\alpha}^{n,k,i}(t))^2 dt \right\}^{\frac{1}{2}},$$

$$\eta_{\text{lin}}^{n,k,i} := \left\{ \sum_{\alpha \in \{\text{n}, \text{w}\}} \tau^n \sum_{K \in \mathcal{T}_h^n} (\eta_{\text{lin},K,\alpha}^{n,k,i})^2 \right\}^{\frac{1}{2}},$$

$$\eta_{\text{alg}}^{n,k,i} := \left\{ \sum_{\alpha \in \{\text{n}, \text{w}\}} \tau^n \sum_{K \in \mathcal{T}_h^n} (\eta_{\text{alg},K,\alpha}^{n,k,i})^2 \right\}^{\frac{1}{2}}$$

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# Cell-centered finite volume scheme

## Cell-centered finite volume scheme

For all  $1 \leq n \leq N$ , look for  $s_{w,h}^n, \bar{p}_{w,h}^n$  such that

$$\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KK'} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KK'}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

$$-\phi \frac{s_{w,K}^n - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KK'} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KK'}}(s_{w,h}^n, \bar{p}_{w,h}^n) = 0,$$

where the fluxes are given by

$$F_{w,e_{KK'}}(s_{w,h}^n, \bar{p}_{w,h}^n) := -\frac{\lambda_w(s_{w,K}^n) + \lambda_w(s_{w,K'}^n)}{2} |\underline{K}| \frac{\bar{p}_{w,K'}^n - \bar{p}_{w,K}^n}{|\mathbf{x}_K - \mathbf{x}_{K'}|} |e_{KK'}|,$$

$$F_{n,e_{KK'}}(s_{w,h}^n, \bar{p}_{w,h}^n) := -\frac{\lambda_n(s_{w,K}^n) + \lambda_n(s_{w,K'}^n)}{2} |\underline{K}| \times \frac{\bar{p}_{w,K'}^n + \pi(s_{w,K'}^n) - (\bar{p}_{w,K}^n + \pi(s_{w,K}^n))}{|\mathbf{x}_K - \mathbf{x}_{K'}|}$$

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# Linearization and algebraic solution

## Linearization step $k$ and algebraic step $i$

Couple  $s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}$  such that

$$\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KK'} \in \mathcal{E}_K^{\text{int}}} F_{w,e_{KK'}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{w,K}^{n,k,i},$$

$$-\phi \frac{s_{w,K}^{n,k,i} - s_{w,K}^{n-1}}{\tau^n} |K| + \sum_{e_{KK'} \in \mathcal{E}_K^{\text{int}}} F_{n,e_{KK'}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) = -R_{n,K}^{n,k,i},$$

where the linearized fluxes are given by

$$\begin{aligned} F_{\alpha,e_{KK'}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}) := & F_{\alpha,e_{KK'}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \\ & + \sum_{M \in \{K, K'\}} \frac{\partial F_{\alpha,e_{KK'}}}{\partial s_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (s_{w,M}^{n,k,i} - s_{w,M}^{n,k-1}) \\ & + \sum_{M \in \{K, K'\}} \frac{\partial F_{\alpha,e_{KK'}}}{\partial \bar{p}_{w,M}}(s_{w,h}^{n,k-1}, \bar{p}_{w,h}^{n,k-1}) \cdot (\bar{p}_{w,M}^{n,k,i} - \bar{p}_{w,M}^{n,k-1}). \end{aligned}$$

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# Fluxes reconstructions and pressure postprocessing

## Fluxes reconstructions

$$(\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KK'}} := F_{\alpha,e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}),$$

$$((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{I}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{e_{KK'}} := F_{\alpha,e_{KK'}}^{\mathbf{k}-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}),$$

$$\mathbf{a}_{\alpha,h}^{n,k,i} := \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{I}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{I}_{\alpha,h}^{n,k,i})$$

## Phase pressures postprocessing

- Piecewise constant  $\bar{p}_{\alpha,h}^{n,k,i}$  postprocessed to piecewise quadratic  $p_{\alpha,h}^{n,k,i}$ :

$$-\lambda_w(s_{w,K}^{n,k,i}) \mathbf{K} \nabla(p_{w,h}^{n,k,i}|_K) = \mathbf{d}_{w,h}^{n,k,i}|_K,$$

$$p_{w,h}^{n,k,i}(\mathbf{x}_K) = \bar{p}_{w,K}^{n,k,i},$$

$$-\lambda_n(s_{w,K}^{n,k,i}) \mathbf{K} \nabla(p_{n,h}^{n,k,i}|_K) = \mathbf{d}_{n,h}^{n,k,i}|_K,$$

$$p_{n,h}^{n,k,i}(\mathbf{x}_K) = \pi(s_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}$$

# Fluxes reconstructions and pressure postprocessing

## Fluxes reconstructions

$$(\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KK'}} := F_{\alpha,e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}),$$

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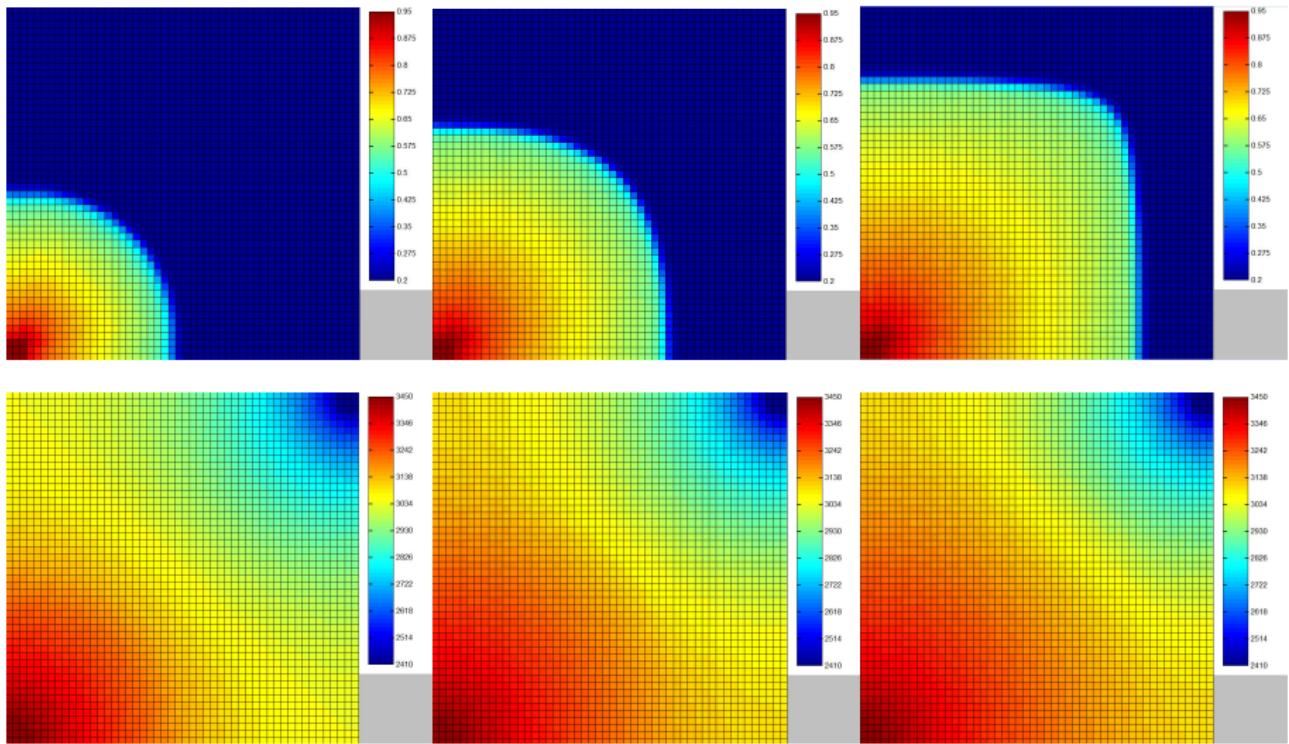
$$-\lambda_w(s_{w,K}^{n,k,i}) \mathbf{K} \nabla (p_{w,h}^{n,k,i}|_K) = \mathbf{d}_{w,h}^{n,k,i}|_K,$$

$$p_{w,h}^{n,k,i}(\mathbf{x}_K) = \bar{p}_{w,K}^{n,k,i},$$

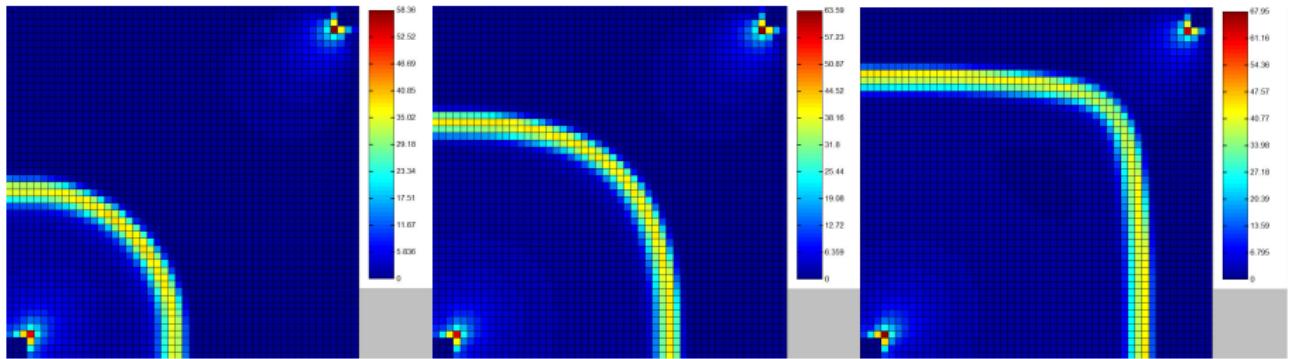
$$-\lambda_n(s_{w,K}^{n,k,i}) \mathbf{K} \nabla (p_{n,h}^{n,k,i}|_K) = \mathbf{d}_{n,h}^{n,k,i}|_K,$$

$$p_{n,h}^{n,k,i}(\mathbf{x}_K) = \pi(s_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}$$

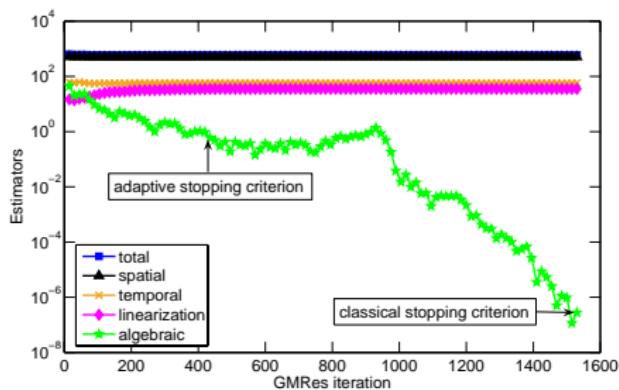
# Water saturation/water pressure evolution



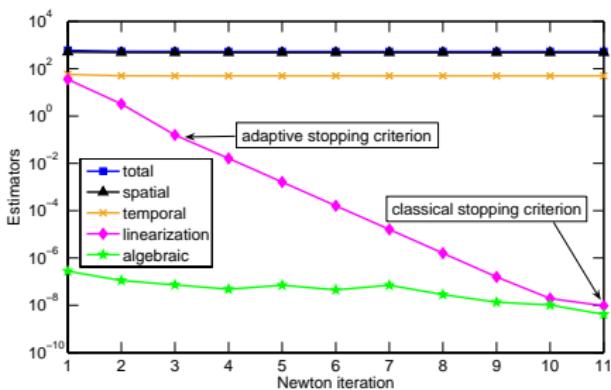
# Estimators evolution



# Estimators and stopping criteria

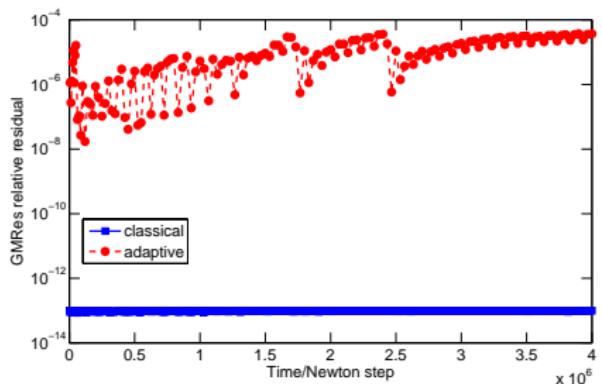


Estimators in function of  
GMRes iterations

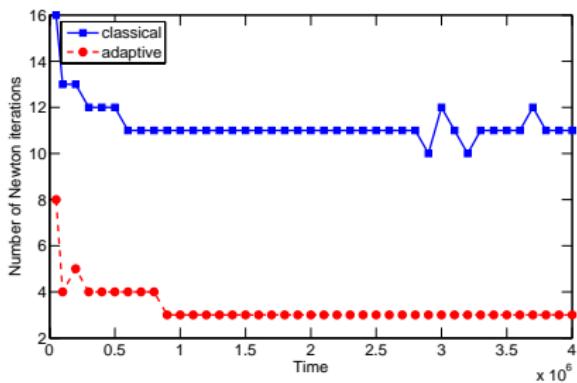


Estimators in function of  
Newton iterations

# GMRes relative residual/Newton iterations

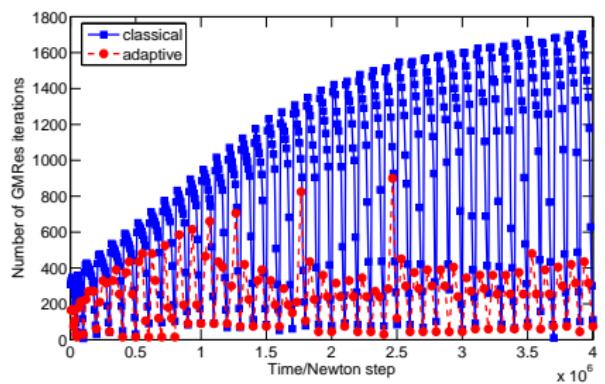


GMRes relative residual

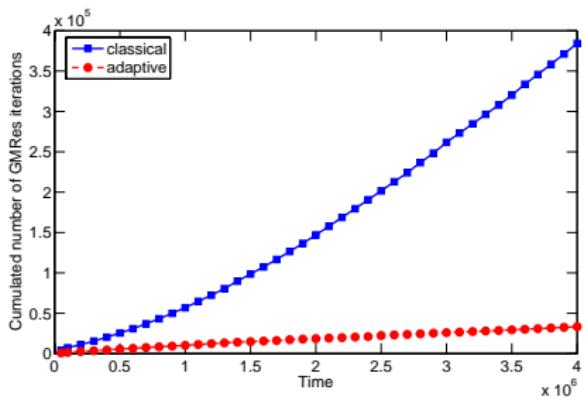


Newton iterations

# GMRes iterations



Per time and Newton step



Cumulated

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# Conclusions

## Entire adaptivity

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

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- other coupled nonlinear systems
- convergence and optimality

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# Bibliography I

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**Merci de votre attention !**