

Adaptive regularization, linearization, and numerical solution of unsteady nonlinear problems

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Outline

- 1 Introduction
- 2 Nonlinear diffusion
 - Quasi-linear elliptic problems
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Applications
 - Numerical results
- 3 The Stefan problem
 - Dual residual and energy norms
 - A posteriori error estimate and its efficiency
 - Numerical results
- 4 Two-phase immiscible incompressible flow
 - Weak solution
 - A posteriori error estimate and its efficiency
 - Applications and numerical results
- 5 Conclusions and future directions

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Numerical approximation of a nonlinear, unsteady PDE

Exact and approximate solution

- let u be the **weak solution** of $A(u) = f$, A **nonlinear**, **unsteady**, posed on $\Omega \times (0, T)$
- let $u_{h\tau}$ be its approximate **numerical solution**,
 $A_{h\tau}(u_{h\tau}) = f_{h\tau}$

Solution algorithm

- introduce a temporal mesh of $(0, T)$ given by the time steps t^n , $0 \leq n \leq N$
- introduce a spatial mesh \mathcal{T}_h^n of Ω on each t^n
- on each t^n , solve a nonlinear algebraic problem
 $A_h^n(u_h^n) = f_h^n$

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Regularization, linearization, and algebraic solution

Regularization

- regularize the nonlinear operator A_h^n by $A_h^{n,\epsilon}$
- choice of ϵ ?

Iterative linearization

- $A_h^{n,\epsilon,k-1} u_h^{n,\epsilon,k} = f_h^{n,k-1}$: $A_h^{n,\epsilon,k-1}$ linear, linearization step k
- when do we stop?

Iterative algebraic solution

- iterative algebraic solver employed: step i approximation $u_h^{n,\epsilon,k,i}$
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Approximate solution

- the approximate solution $u_h^{n,\epsilon,k,i}$ that we have as an outcome does not solve $A_h^n(u_h^n) = f_h^n$
- how big is the overall error $\|u - u_{h\tau}^{\epsilon,k,i}\|_{\Omega \times (0,T)}$?

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- give a **guaranteed**, **robust**, and **tight** upper bound on the overall error $\|u - u_{h\tau}^{\epsilon,k,i}\|_{\Omega \times (0, T)}$
- **distinguish** the different **error components** (algebraic, linearization, regularization, spatial, temporal)
- **stop** the **iterative solvers** whenever algebraic/linearization errors do not affect the overall error significantly
- **adjust** the **regularization parameter** so that it does not to affect the overall error significantly
- **equilibrate** the space and time **error components**

Benefits

- **optimal computable overall error bound**
- **improvement of approximation precision**
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Previous results

Stopping criteria

- engineering literature, since 1950's
- Becker, Johnson, and Rannacher (1995), multigrid solver
- Maday and Patera (2000), linear functional errors
- Arioli (2000's), general algebraic solvers

Inexact Newton method

- Eisenstat and Walker (1990's)
- Moret (1989)

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- Ladevèze (since 1980's)
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Nonlinear steady problems

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- Chaillou and Suri (2006, 2007), linearization errors
- Kim (2007), guaranteed estimates, loc. cons. methods

Linear unsteady problems

- Bieterman and Babuška (1982), introduction
- Verfürth (2003), efficiency, robustness wrt the final time

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Quasi-linear elliptic problem

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

- 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

$$A(u) = f \text{ in } V'$$

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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

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

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

- 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

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

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Approximate solution

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- $V(\mathcal{T}_h) := \{v \in L^p(\Omega), v|_K \in W^{1,p}(K) \quad \forall K \in \mathcal{T}_h\}$

Error measure

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

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

- 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

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

Approximate solution and error measure

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A posteriori error estimate

Assumption A (Total flux reconstruction)

There exists a *flux reconstruction* $\mathbf{t}_h^{k,i} \in \mathbf{H}^q(\operatorname{div}, \Omega)$ 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. $(f_h, \mathbf{1})_K = (f, \mathbf{1})_K \quad \forall K \in \mathcal{T}_h$.

Theorem (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 $\rho_h^{k,i}$.

A posteriori error estimate

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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 different 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

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

Estimate distinguishing different error components

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Estimators

- *discretization estimator*

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

- *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*

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

- *data oscillation estimator*

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

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

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Stopping criteria

Global stopping criteria

- stop whenever:

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

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

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

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

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

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

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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

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

Global efficiency

Theorem (Global efficiency)

Let the mesh \mathcal{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 σ and q .

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

$$\begin{aligned} & \eta_{\text{disc},K}^{k,i} + \eta_{\text{lin},K}^{k,i} + \eta_{\text{alg},K}^{k,i} + \eta_{\text{rem},K}^{k,i} \\ & \lesssim \mathcal{J}_{u,\mathfrak{T}_K}^{\text{up}}(u_h^{k,i}) + \eta_{\text{quad},\mathfrak{T}_K}^{k,i} + \eta_{\text{osc},\mathfrak{T}_K}^{k,i} \end{aligned}$$

for all $K \in \mathcal{T}_h$.

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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

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

- Do ν additional steps of the algebraic solver, yielding

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

- 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

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

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

- 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

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Example: nonconforming finite elements for the p -Laplacian

Discretization

Find $u_h \in V_h$ 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
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$$\mathcal{A}(U) = F$$

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Linearization

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Find $u_h^k \in V_h$ such that

$$(\sigma^{k-1}(\nabla u_h^k), \nabla \psi_e) = (f_h, \psi_e) \quad \forall e \in \mathcal{E}_h^{\text{int}}.$$

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

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

- Newton linearization

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

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Algebraic solution

Algebraic solution

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

$$(\sigma^{k-1}(\nabla u_h^{k,i}), \nabla \psi_e) = (f_h, \psi_e) - R_e^{k,i} \quad \forall e \in \mathcal{E}_h^{\text{int}}.$$

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

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

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

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

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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.
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- $\mathbf{d}_h^{k,i}$ close to $\sigma(\nabla u_h^{k,i})$
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Summary

Discretization methods

- nonconforming finite elements
- discontinuous Galerkin
- finite elements
- 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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Numerical experiment I

Model problem

- p -Laplacian

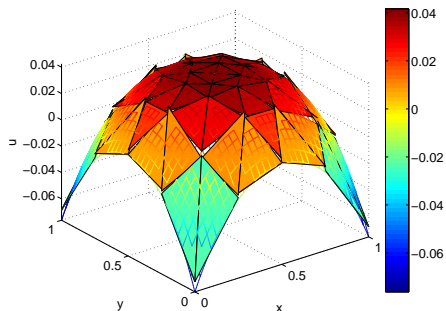
$$\begin{aligned}\nabla \cdot (|\nabla u|^{p-2} \nabla u) &= f && \text{in } \Omega, \\ u &= u_0 && \text{on } \partial\Omega\end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

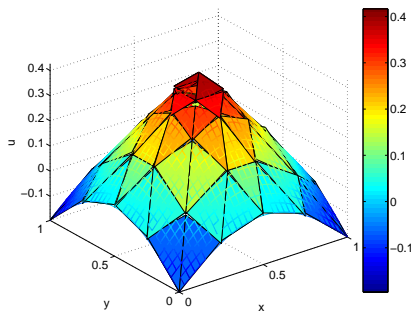
$$u(x, y) = -\frac{p-1}{p} \left((x - \frac{1}{2})^2 + (y - \frac{1}{2})^2 \right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p} \left(\frac{1}{2} \right)^{\frac{p}{p-1}}$$

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

Analytical and approximate solutions

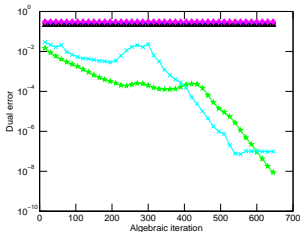


Case $p = 1.5$

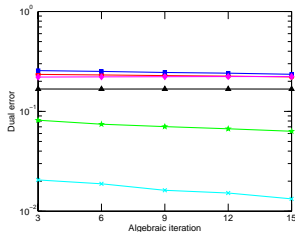


Case $p = 10$

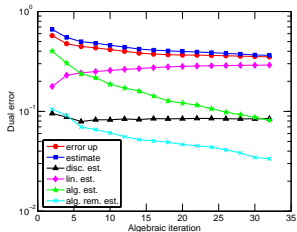
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

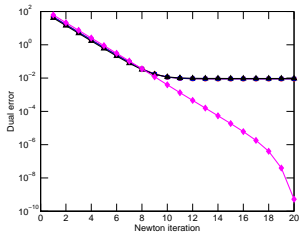


inexact Newton

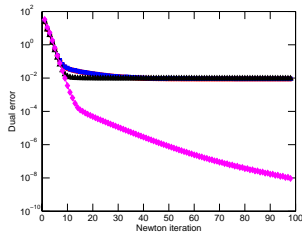


ad. inexact Newton

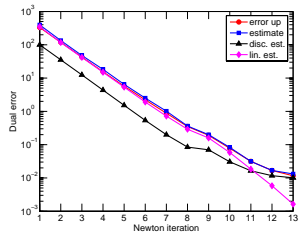
Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh



Newton

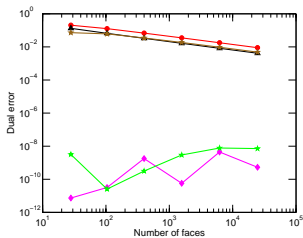


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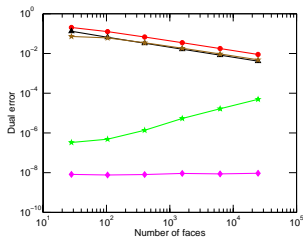


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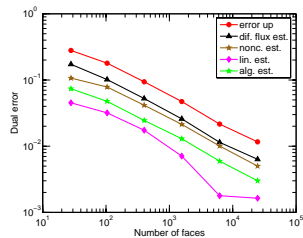
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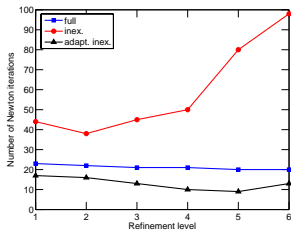


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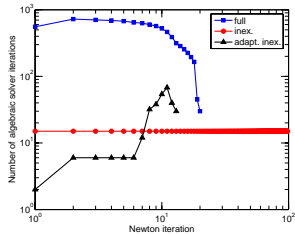


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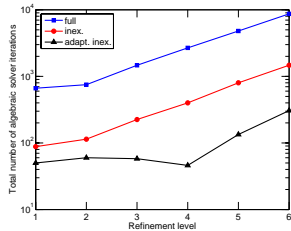
Newton and algebraic iterations, $p = 10$



Newton it. / refinement

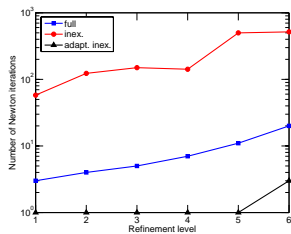


alg. it. / Newton step

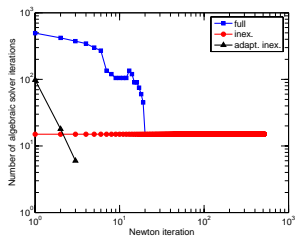


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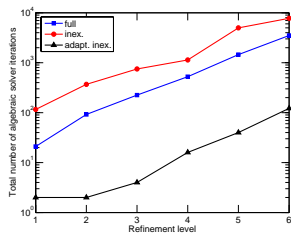
Newton and algebraic iterations, $p = 1.5$



Newton it. / refinement



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Numerical experiment II

Model problem

- p -Laplacian

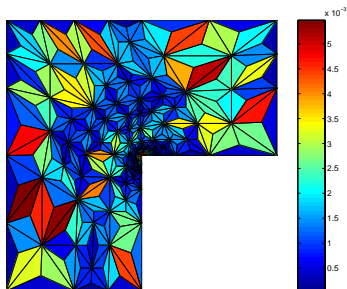
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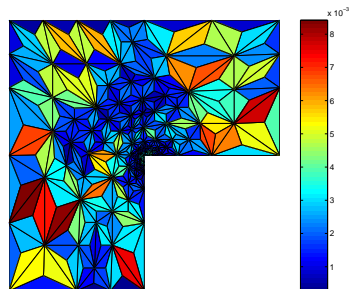
$$u(r, \theta) = r^{\frac{7}{8}} \sin(\theta \frac{7}{8})$$

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

Error distribution on an adaptively refined mesh

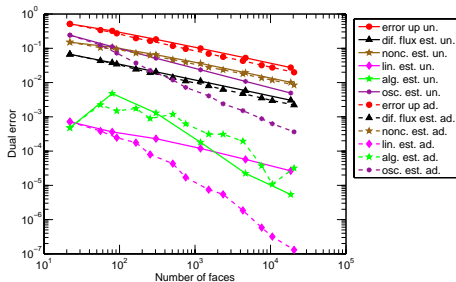


Estimated error distribution

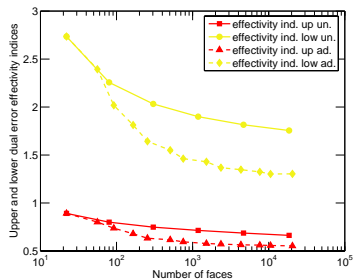


Exact error distribution

Estimated and actual errors and the effectivity index

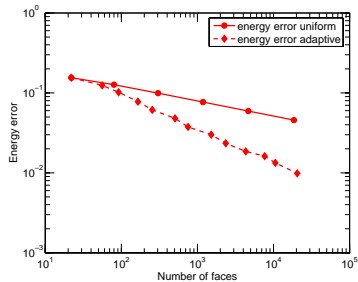


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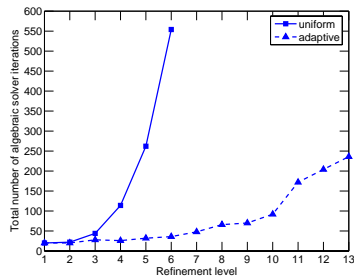


Effectivity index

Energy error and overall performance



Energy error



Overall performance

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The Stefan problem

The Stefan problem

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

Nomenclature

- u enthalpy, $\beta(u)$ temperature
- β : L_β -Lipschitz continuous, $\beta(s) = 0$ in $(0, 1)$, strictly increasing otherwise
- phase change, degenerate parabolic problem
- $u_0 \in L^2(\Omega)$, $f \in L^2(0, T; L^2(\Omega))$

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Residual and its dual norm

Functional spaces

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

Weak formulation

$$u \in Z \quad \text{with } \beta(u) \in X$$

$$u(\cdot, 0) = u_0 \quad \text{in } \Omega$$

$$\langle \partial_t u, \varphi \rangle(t) + (\nabla \beta(u), \nabla \varphi)(t) = (f, \varphi)(t) \quad \forall \varphi \in H_0^1(\Omega) \quad \text{a.e. } t \in (0, T)$$

Residual for $u_{h\tau} \in Z$ such that $\beta(u_{h\tau}) \in X$

$$\langle \mathcal{R}(u_{h\tau}), \varphi \rangle_{X', X} = \int_0^T \{ \langle \partial_t(u - u_{h\tau}), \varphi \rangle + (\nabla \beta(u) - \nabla \beta(u_{h\tau}), \nabla \varphi) \} (t) dt,$$

$$\varphi \in X$$

Dual norm of the residual

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

Residual and its dual norm

Functional spaces

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

Weak formulation

$$u \in Z \quad \text{with } \beta(u) \in X$$

$$u(\cdot, 0) = u_0 \quad \text{in } \Omega$$

$$\langle \partial_t u, \varphi \rangle(t) + (\nabla \beta(u), \nabla \varphi)(t) = (f, \varphi)(t) \quad \forall \varphi \in H_0^1(\Omega) \quad \text{a.e. } t \in (0, T)$$

Residual for $u_{h\tau} \in Z$ such that $\beta(u_{h\tau}) \in X$

$$\langle \mathcal{R}(u_{h\tau}), \varphi \rangle_{X', X} = \int_0^T \{ \langle \partial_t(u - u_{h\tau}), \varphi \rangle + (\nabla \beta(u) - \nabla \beta(u_{h\tau}), \nabla \varphi) \} (t) dt,$$

$$\varphi \in X$$

Dual norm of the residual

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

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Time-localization of the dual norm of the residual

Time interval I_n

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L^2 in time ...

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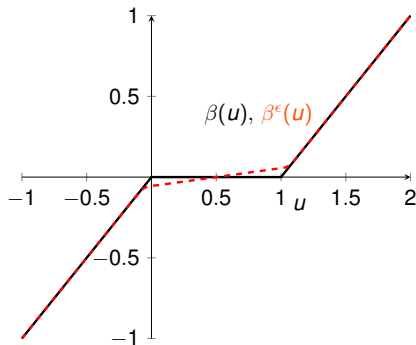
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Practice: regularization

Regularization with a parameter ϵ



Practice: questions

Discretization



Question (Stopping and balancing criteria)

- What is a good *choice* of the
 - regularization parameter ϵ ?
 - time step?
 - space mesh?
- What is a good *stopping criterion* for the
 - nonlinear solver?
 - linear solver?

Question (Error)

- How big is the error $\|u|_{I_n} - u_{h\tau}^{n,\epsilon,k,i}\|$ on time step n , space mesh \mathcal{T}_h^n , for the regularization parameter ϵ , Newton step k , and algebraic solver step i ? How *big* are the *individual components*? How is error *distributed in time and space*?

Practice: questions

Discretization

- ...

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A posteriori estimate and its efficiency

Theorem (Estimate and its efficiency)

There holds

$$\begin{aligned} & \|\mathcal{R}(u_{h\tau})\|_{X'} + \|u_0 - u_{h\tau}(0)\|_{H^{-1}(\Omega)} \\ & \leq \left\{ \sum_{n=1}^N \int_{I_n} \sum_{K \in \mathcal{T}_h^n} (\eta_{R,K}^n + \eta_{F,K}^n)^2 \right\}^{\frac{1}{2}} + \eta_{IC} \\ & \lesssim \|\mathcal{R}(u_{h\tau})\|_{X'} + \|u_0 - u_{h\tau}(0)\|_{H^{-1}(\Omega)}, \end{aligned}$$

with

$$\begin{aligned} \eta_{R,K}^n &:= C_{P,K} h_K \|f^n - \partial_t u_{h\tau} - \nabla \cdot \mathbf{t}_h^n\|_K, \\ \eta_{F,K}^n(t) &:= \|\nabla \beta(u_{h\tau}(t)) + \mathbf{t}_h^n\|_K, \\ \eta_{IC} &:= \|u_0 - u_{h\tau}(0)\|_{H^{-1}(\Omega)}. \end{aligned}$$

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Distinguishing the different error components

Theorem (An estimate distinguishing the error components)

For time n , linearization k , and regularization ϵ , there holds

$$\|\mathcal{R}(u_{h\tau}^{n,\epsilon,k})\|_{X',I_n} \leq \eta_{\text{sp}}^{n,\epsilon,k} + \eta_{\text{tm}}^{n,\epsilon,k} + \eta_{\text{lin}}^{n,\epsilon,k} + \eta_{\text{reg}}^{n,\epsilon,k}.$$

- $\sigma^{n,\epsilon,k}$ a scheme linearized flux (not $\mathbf{H}(\text{div}, \Omega)$), $\mathbf{t}^{n,\epsilon,k}$ reconstructed $\mathbf{H}(\text{div}, \Omega)$ flux, Π^n interpolation

$$(\eta_{\text{sp}}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{T}_h^n} \left(\eta_{\mathbf{R},K}^{n,\epsilon,k} + \|\sigma^{n,\epsilon,k} + \mathbf{t}^{n,\epsilon,k}\|_K \right)^2,$$

$$(\eta_{\text{tm}}^{n,\epsilon,k})^2 := \int_{I_n} \sum_{K \in \mathcal{T}_h^n} \|\nabla \Pi^n \beta(u_{h\tau}^{\epsilon,k})(t) - \nabla \Pi^n \beta(u_{h\tau}^{\epsilon,k})(t^n)\|_K^2 dt,$$

$$(\eta_{\text{lin}}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{T}_h^n} \|\nabla \Pi^n \beta_\epsilon(u_{h\tau}^{\epsilon,k})(t^n) - \sigma^{n,\epsilon,k}\|_K^2,$$

$$(\eta_{\text{reg}}^{n,\epsilon,k})^2 := \tau^n \sum_{K \in \mathcal{T}_h^n} \|\nabla \Pi^n \beta(u_{h\tau}^{\epsilon,k})(t^n) - \nabla \Pi^n \beta_\epsilon(u_{h\tau}^{\epsilon,k})(t^n)\|_K^2$$

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Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

$$\begin{aligned} & \frac{L_\beta}{2} \|u - u_{h_T}\|_{X'}^2 + \|\beta(u) - \beta(u_{h_T})\|_{Q_T}^2 \\ & \leq \frac{L_\beta}{2} (2e^T - 1) \left(\|\mathcal{R}(u_{h_T})\|_{X'}^2 + \|(u - u_{h_T})(0)\|_{H^{-1}(\Omega)}^2 \right) \end{aligned}$$

Theorem (Temperature and enthalpy errors, tight Gronwall)

Let $u_{h_T} \in Z$ be such that $\beta(u_{h_T}) \in X$ be arbitrary. There holds

$$\begin{aligned} & \frac{L_\beta}{2} \|u - u_{h_T}\|_{X'}^2 + \frac{L_\beta}{2} \|(u - u_{h_T})(T)\|_{H^{-1}(\Omega)}^2 + \|\beta(u) - \beta(u_{h_T})\|_{Q_T}^2 \\ & + 2 \int_0^T \left(\|\beta(u) - \beta(u_{h_T})\|_{Q_t}^2 + \int_0^t \|\beta(u) - \beta(u_{h_T})\|_{Q_s}^2 e^{t-s} ds \right) dt \\ & \leq \frac{L_\beta}{2} \left\{ (2e^T - 1) \|(u - u_{h_T})(0)\|_{H^{-1}(\Omega)}^2 + \|\mathcal{R}(u_{h_T})\|_{X'}^2 \right. \\ & \left. + 2 \int_0^T \left(\|\mathcal{R}(u_{h_T})\|_{X'_t}^2 + \int_0^t \|\mathcal{R}(u_{h_T})\|_{X'_s}^2 e^{t-s} ds \right) dt \right\}. \end{aligned}$$

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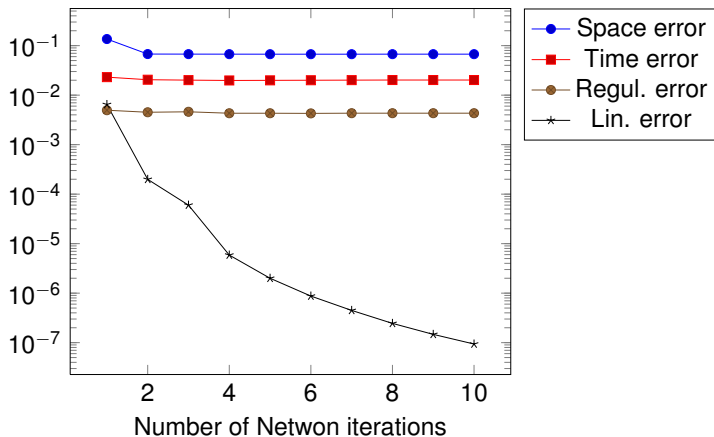
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Linearization stopping criterion

Linearization stopping criterion

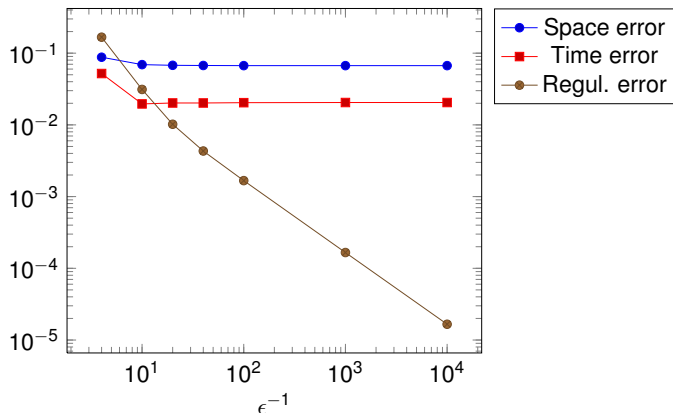
$$\eta_{\text{lin}}^{n,\epsilon,k} \leq \gamma_{\text{lin}} (\eta_{\text{sp}}^{n,\epsilon,k} + \eta_{\text{tm}}^{n,\epsilon,k} + \eta_{\text{reg}}^{n,\epsilon,k})$$



Regularization stopping criterion

Regularization stopping criterion

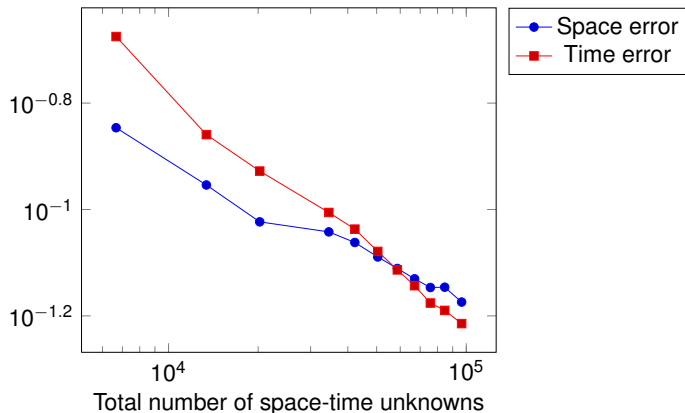
$$\eta_{\text{reg}}^{n,\epsilon,k} \leq \gamma_{\text{reg}} (\eta_{\text{sp}}^{n,\epsilon,k} + \eta_{\text{tm}}^{n,\epsilon,k})$$



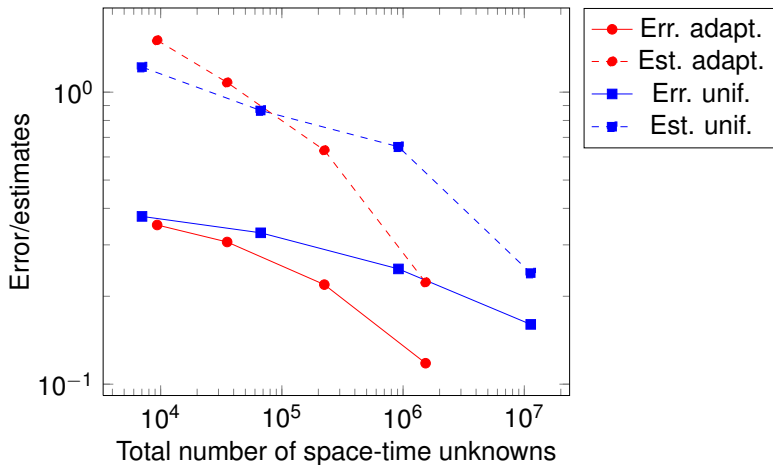
Equilibrating time and space errors

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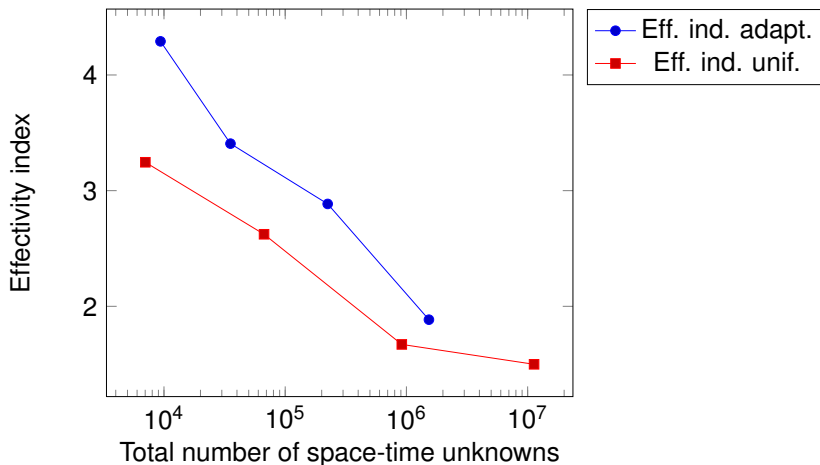
$$\gamma_{\min} \eta_{\text{sp}}^{\epsilon, n, k} \leq \eta_{\text{tm}}^{\epsilon, n, k} \leq \gamma_{\max} \eta_{\text{sp}}^{\epsilon, n, k}$$



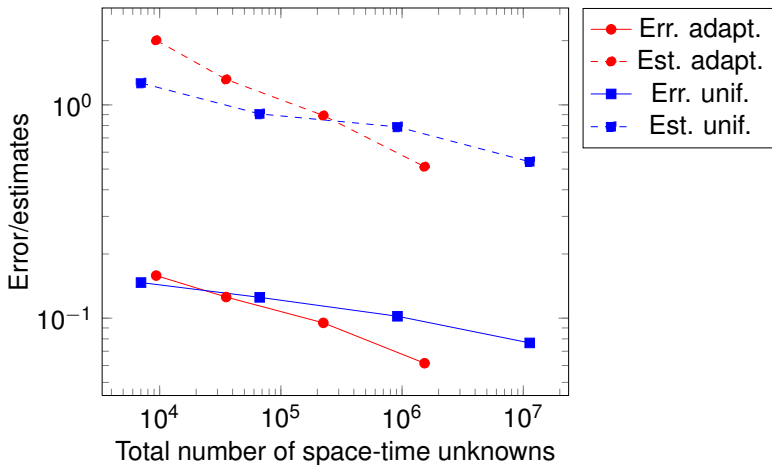
Error and estimate (dual norm)



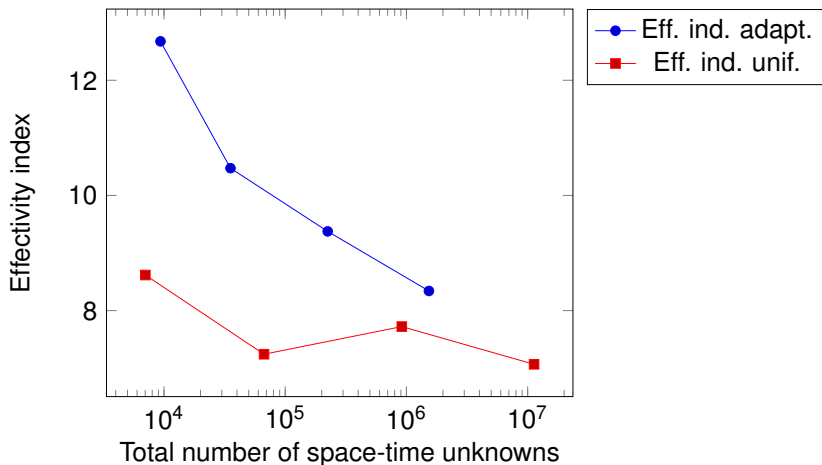
Effectivity indices (dual norm)



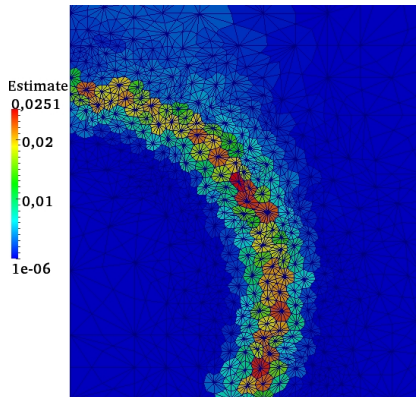
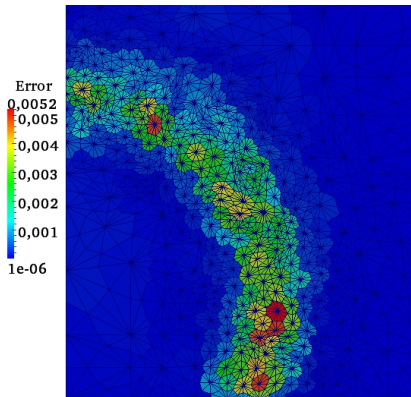
Error and estimate (energy norm)



Effectivity indices (energy norm)



Actual and estimated error distribution



Computational efficiency

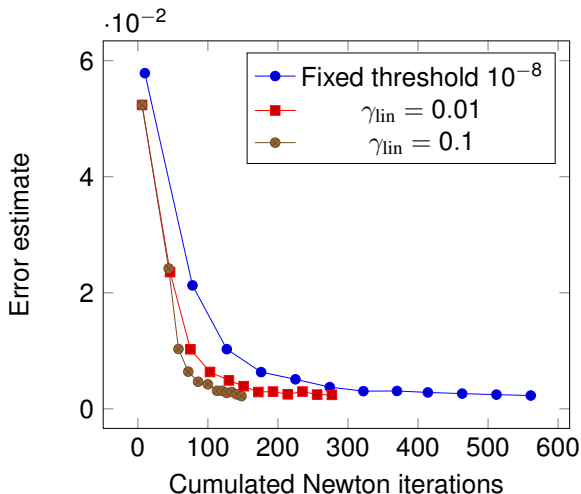


Figure: Number of cumulated Newton iterations vs. error estimate

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Two-phase flow

The model

$$\begin{aligned} \partial_t \mathbf{s}_\alpha + \nabla \cdot \mathbf{u}_\alpha &= q_\alpha(\mathbf{s}_\alpha), & \alpha \in \{\mathbf{n}, \mathbf{w}\}, \\ \mathbf{u}_\alpha &= -\underline{\mathbf{K}} \eta_\alpha(\mathbf{s}_\alpha) \nabla p_\alpha, & \alpha \in \{\mathbf{n}, \mathbf{w}\}, \\ \mathbf{s}_\mathbf{n} + \mathbf{s}_\mathbf{w} &= \mathbf{1}, \\ \rho_\mathbf{n} - \rho_\mathbf{w} &= \pi(\mathbf{s}_\mathbf{n}) \end{aligned}$$

- two immiscible, incompressible fluids
- $p_\mathbf{n}, p_\mathbf{w}$: unknown nonwetting and wetting phase pressures
- $s_\mathbf{n}, s_\mathbf{w}$: unknown nonwetting and wetting phase saturations
- $\pi(\cdot)$: the nonlinear capillary pressure function
- $\eta_\mathbf{n}(\cdot), \eta_\mathbf{w}(\cdot)$: the nonlinear phase mobilities functions
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Notation and transformations

Notation and transformations

- $s := s_n$



$$f(s) := \frac{\eta_n(s)}{\eta_n(s) + \eta_w(1-s)}, \quad \lambda(s) := \eta_w(1-s)f(s)$$

- Kirchhoff transform

$$\varphi(s) := \int_0^s \lambda(a) \pi'(a) da$$

- global pressure

$$P := P(s, p_n) := p_n - \int_0^{\pi(s)} \frac{\eta_w(1 - \pi^{-1}(a))}{\eta_n(\pi^{-1}(a)) + \eta_w(1 - \pi^{-1}(a))} da$$

- $M(s) := \eta_w(1-s) + \eta_n(s)$

- $q_t(s) := q_n(s) + q_w(1-s)$

- $f, \lambda, \varphi, P, M, q_t$ only needed for the theoretical analysis, not in the scheme

- s^0 : initial condition

- \bar{s}, \bar{P} : Dirichlet boundary conditions

Notation and transformations

Notation and transformations

- $s := s_n$



$$f(s) := \frac{\eta_n(s)}{\eta_n(s) + \eta_w(1-s)}, \quad \lambda(s) := \eta_w(1-s)f(s)$$

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Weak formulation

Functional space for the weak solution

$$\mathcal{E} := \{ (s, P) \mid s \in C([0, T]; L^2(\Omega)), \partial_t s \in L^2((0, T); H^{-1}(\Omega)), \\ \varphi(s) - \varphi(\bar{s}) \in L^2((0, T); H_0^1(\Omega)), P - \bar{P} \in L^2((0, T); H_0^1(\Omega)) \}$$

Definition (Weak solution)

A weak solution is a pair $(s, P) \in \mathcal{E}$ such that $s(\cdot, 0) = s^0$ and for all $\psi \in L^2((0, T); H_0^1(\Omega))$,

$$\int_0^T \langle \partial_t s(\cdot, \theta); \psi(\cdot, \theta) \rangle_{H^{-1}, H_0^1} d\theta + \iint_{Q_T} \underline{\mathbf{K}}(\eta_n(s)) \nabla P + \nabla \varphi(s) \cdot \nabla \psi \, d\mathbf{x} d\theta \\ = \iint_{Q_T} q_n(s) \psi \, d\mathbf{x} d\theta, \\ \iint_{Q_T} \underline{\mathbf{K}} M(s) \nabla P \cdot \nabla \psi \, d\mathbf{x} d\theta = \iint_{Q_T} q_t(s) \psi \, d\mathbf{x} d\theta.$$

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- 2 Nonlinear diffusion
 - Quasi-linear elliptic problems
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Applications
 - Numerical results
- 3 The Stefan problem
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 - Weak solution
 - **A posteriori error estimate and its efficiency**
 - Applications and numerical results
- 5 Conclusions and future directions

A posteriori error estimate

Functional space for the approximate solution

$$\mathcal{E}_\tau := \left\{ (s, P) \mid s \in V_\tau, \text{ pw affine-in-time subspace of } \mathcal{C}([0, T]; L^2(\Omega)), \right. \\ \left. \varphi(s) - \varphi(\bar{s}) \in L^2((0, T); H_0^1(\Omega)), P - \bar{P} \in L^2((0, T); H_0^1(\Omega)) \right\}$$

Theorem (A posteriori error estimate)

Let (s, P) be the weak solution. Let $(s_{h\tau}, P_{h\tau}) \in \mathcal{E}_\tau$ be arbitrary. Then there exists $C > 0$ such that

$$\|s_{h\tau} - s\|_{L^2(0, T; H^{-1}(\Omega))}^2 + \|P_{h\tau} - P\|_{L^2(0, T; H_0^1(\Omega))}^2 + \|\varphi(s_{h\tau}) - \varphi(s)\|_{L^2(Q_T)}^2 \\ \leq C \|s_{h\tau}(\cdot, 0) - s^0\|_{H^{-1}(\Omega)}^2 \\ + C (\|\mathcal{R}_n^n(s_{h\tau}, P_{h\tau})\|^2 + \|\mathcal{R}_t^n(s_{h\tau}, P_{h\tau})\|^2).$$

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Distinguishing different error components

Theorem (Distinguishing different error components)

Consider

- *time step* n
- *linearization step* k
- *iterative algebraic solver step* i

& approximations $(s_{h\tau}^{k,i}, P_{h\tau}^{k,i})$. Let there exist *equilibrated fluxes reconstructions* $u_{\alpha,h}^{n,k,i}$ for each phase $\alpha \in n, w$. Split them as

$$u_{\alpha,h}^{n,k,i} := d_{\alpha,h}^{n,k,i} + l_{\alpha,h}^{n,k,i} + a_{\alpha,h}^{n,k,i}, \alpha \in \{n, w\}.$$

Then

$$\begin{aligned} & (\| \mathcal{R}_n^n(s_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}) \| + \| \mathcal{R}_t^n(s_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}) \|)^2 \\ & \leq \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i}. \end{aligned}$$

Moreover, if $\eta_{tm}^{n,k,i}$, $\eta_{lin}^{n,k,i}$, and $\eta_{alg}^{n,k,i}$ do not dominate, then

$$\begin{aligned} & \eta_{sp}^{n,k,i} + \eta_{tm}^{n,k,i} + \eta_{lin}^{n,k,i} + \eta_{alg}^{n,k,i} \\ & \leq C (\| \mathcal{R}_n^n(s_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}) \| + \| \mathcal{R}_t^n(s_{h\tau}^{n,k,i}, P_{h\tau}^{n,k,i}) \|)^2. \end{aligned}$$

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Estimators

- spatial estimators*

$$\eta_{\text{sp},n,D}^{n,k,i} := \|\mathbf{d}_{n,h}^{n,k,i} - \underline{\mathbf{K}}(\eta(\mathbf{s}_{h\tau}^{n,k,i})\nabla P_{h\tau}^{n,k,i} + \nabla\varphi(\mathbf{s}_{h\tau}^{n,k,i}))(t^n)\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)},$$

$$\eta_{\text{sp},t,D}^{n,k,i} := \|\mathbf{d}_{t,h}^{n,k,i} - \underline{\mathbf{K}}M(\mathbf{s}_{h\tau}^{n,k,i})\nabla P_{h\tau}^{n,k,i}(t^n)\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)}$$

- temporal estimators*

$$\eta_{\text{tm},n,D}^{n,k,i}(t) := \|\underline{\mathbf{K}}(\eta(\mathbf{s}_{h\tau}^{n,k,i})\nabla P_{h\tau}^{n,k,i} + \nabla\varphi(\mathbf{s}_{h\tau}^{n,k,i}))(t - t^n)\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)},$$

$$\eta_{\text{tm},t,D}^{n,k,i}(t) := \|\underline{\mathbf{K}}M(\mathbf{s}_{h\tau}^{n,k,i})\nabla P_{h\tau}^{n,k,i}(t - t^n)\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)}$$

- linearization estimators*

$$\eta_{\text{lin},n,D}^{n,k,i} := \|\mathbf{l}_{n,h}^{n,k,i}\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)},$$

$$\eta_{\text{lin},t,D}^{n,k,i} := \|\mathbf{l}_{t,h}^{n,k,i}\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)}$$

- algebraic estimators*

$$\eta_{\text{alg},n,D}^{n,k,i} := \|\mathbf{a}_{n,h}^{n,k,i}\|_{\underline{\mathbf{K}}^{-\frac{1}{2}};L^2(D)},$$

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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

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

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where the fluxes are given by

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

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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

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

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

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

Fluxes reconstructions and pressure postprocessing

Fluxes reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KK'}} &:= F_{\alpha, e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{e_{KK'}} &:= F_{\alpha, e_{KK'}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

Phase pressures postprocessing

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

$$\begin{aligned}
 -\eta_{r,w}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{w,h}^{n,k,i}|_K) &= \mathbf{d}_{w,h}^{n,k,i}|_K, \\
 p_{w,h}^{n,k,i}(\mathbf{x}_K) &= \bar{p}_{w,K}^{n,k,i},
 \end{aligned}$$

$$\begin{aligned}
 -\eta_{r,n}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla(p_{n,h}^{n,k,i}|_K) &= \mathbf{d}_{n,h}^{n,k,i}|_K, \\
 p_{n,h}^{n,k,i}(\mathbf{x}_K) &= \pi(s_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}
 \end{aligned}$$

Fluxes reconstructions and pressure postprocessing

Fluxes reconstructions

$$\begin{aligned}
 (\mathbf{d}_{\alpha,h}^{n,k,i} \cdot \mathbf{n}_K, 1)_{e_{KK'}} &:= F_{\alpha, e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 ((\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i}) \cdot \mathbf{n}_K, 1)_{e_{KK'}} &:= F_{\alpha, e_{KK'}}^{k-1}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}), \\
 \mathbf{a}_{\alpha,h}^{n,k,i} &:= \mathbf{d}_{\alpha,h}^{n,k,i+\nu} + \mathbf{l}_{\alpha,h}^{n,k,i+\nu} - (\mathbf{d}_{\alpha,h}^{n,k,i} + \mathbf{l}_{\alpha,h}^{n,k,i})
 \end{aligned}$$

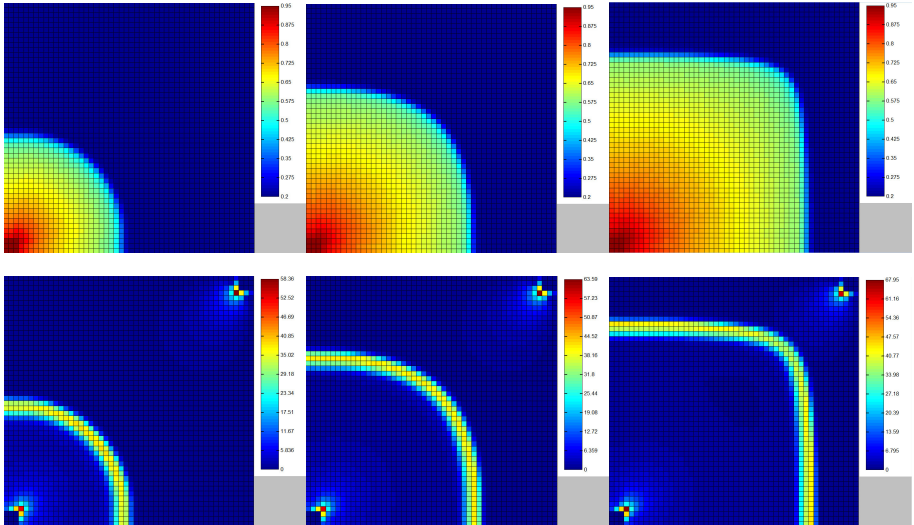
Phase pressures postprocessing

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

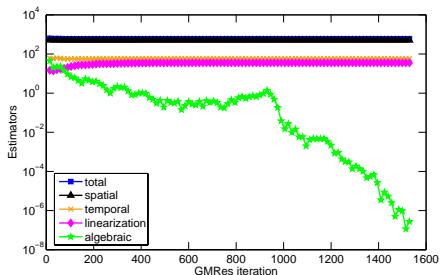
$$\begin{aligned}
 -\eta_{r,w}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla (p_{w,h}^{n,k,i}|_K) &= \mathbf{d}_{w,h}^{n,k,i}|_K, \\
 p_{w,h}^{n,k,i}(\mathbf{x}_K) &= \bar{p}_{w,K}^{n,k,i},
 \end{aligned}$$

$$\begin{aligned}
 -\eta_{r,n}(s_{w,K}^{n,k,i}) \underline{\mathbf{K}} \nabla (p_{n,h}^{n,k,i}|_K) &= \mathbf{d}_{n,h}^{n,k,i}|_K, \\
 p_{n,h}^{n,k,i}(\mathbf{x}_K) &= \pi(s_{w,K}^{n,k,i}) + \bar{p}_{w,K}^{n,k,i}
 \end{aligned}$$

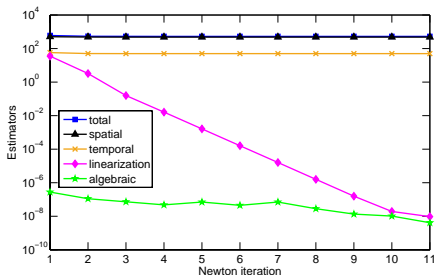
Water saturation/estimators evolution



Estimators and stopping criteria

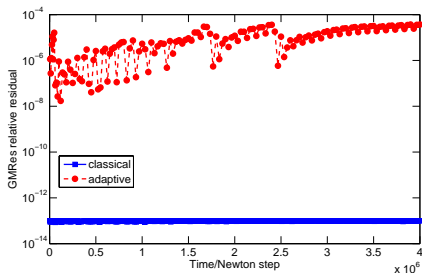


Estimators in function of
GMRes iterations

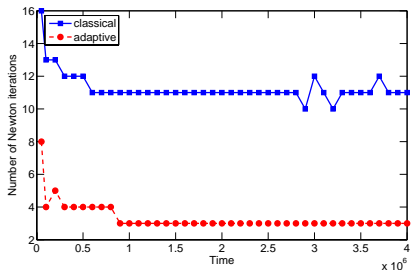


Estimators in function of
Newton iterations

GMRes relative residual/Newton iterations

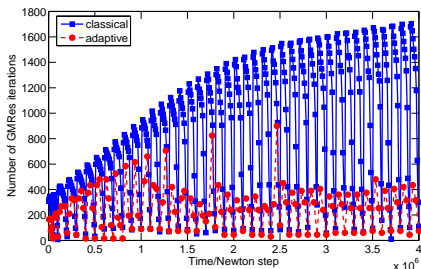


GMRes relative residual

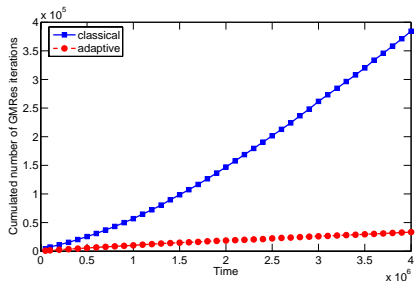


Newton iterations

GMRes iterations



Per time and Newton step



Cumulated

Vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

Explicit saturation equation on step k

$$s_{w,D}^{n,k} := \frac{\tau^n}{\phi |D|} \left(\eta_{r,w}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} + s_{w,D}^{n-1} \quad \forall D \in \mathcal{D}_h^{\text{int},n}$$

Vertex-centered finite volumes

Implicit pressure equation on step k

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} = 0 \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

Explicit saturation equation on step k

$$s_{w,D}^{n,k} := \frac{\tau^n}{\phi |D|} \left(\eta_{r,w}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k} \cdot \mathbf{n}_D, 1 \right)_{\partial D \setminus \partial \Omega} + s_{w,D}^{n-1} \quad \forall D \in \mathcal{D}_h^{\text{int},n}$$

Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$\begin{aligned}
 & - \left((\eta_{r,w}(s_{w,h}^{n,k-1}) + \eta_{r,n}(s_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(s_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} = -R_{t,D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

$$s_{w,D}^{n,k,i} := \frac{\tau^n}{\phi |D|} \left(\eta_{r,w}(s_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} + s_{w,D}^{n-1}$$

Linearization and algebraic solution

Iterative coupling step k and algebraic step i

$$\begin{aligned}
 & - \left((\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\
 & \quad \left. + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(\mathbf{s}_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} = -R_{t,D}^{n,k,i} \quad \forall D \in \mathcal{D}_h^{\text{int},n}
 \end{aligned}$$

$$\mathbf{s}_{w,D}^{n,k,i} := \frac{\tau^n}{\phi |D|} \left(\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1} \right)_{\partial D \setminus \partial \Omega} + \mathbf{s}_{w,D}^{n-1}$$

Fluxes reconstructions

Total fluxes

$$(\mathbf{d}_{t,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e := - \left((\eta_{r,w}(\mathbf{s}_{w,h}^{n,k,i}) + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k,i})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla \bar{\pi}(\mathbf{s}_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1} \right)_e,$$

$$((\mathbf{d}_{t,h}^{n,k,i} + \mathbf{l}_{t,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1})_e := - \left((\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla \bar{\pi}(\mathbf{s}_{w,h}^{n,k-1}) \cdot \mathbf{n}_D, \mathbf{1} \right)_e,$$

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

Wetting fluxes

$$(\mathbf{d}_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e := - (\eta_{r,w}(\mathbf{s}_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e,$$

$$((\mathbf{d}_{w,h}^{n,k,i} + \mathbf{l}_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1})_e := - (\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e,$$

$$\mathbf{a}_{w,h}^{n,k,i} := 0$$

Fluxes reconstructions

Total fluxes

$$(\mathbf{d}_{t,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e := - \left((\eta_{r,w}(\mathbf{s}_{w,h}^{n,k,i}) + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k,i})) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D \right. \\ \left. + \eta_{r,n}(\mathbf{s}_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla \bar{\pi}(\mathbf{s}_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1} \right)_e,$$

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

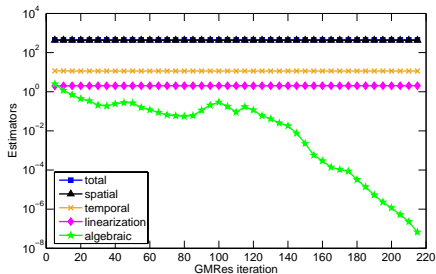
Wetting fluxes

$$(\mathbf{d}_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e := - (\eta_{r,w}(\mathbf{s}_{w,h}^{n,k,i}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e,$$

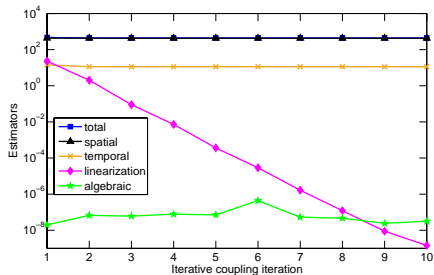
$$((\mathbf{d}_{w,h}^{n,k,i} + \mathbf{l}_{w,h}^{n,k,i}) \cdot \mathbf{n}_D, \mathbf{1})_e := - (\eta_{r,w}(\mathbf{s}_{w,h}^{n,k-1}) \underline{\mathbf{K}} \nabla p_{w,h}^{n,k,i} \cdot \mathbf{n}_D, \mathbf{1})_e,$$

$$\mathbf{a}_{w,h}^{n,k,i} := 0$$

Estimators and stopping criteria

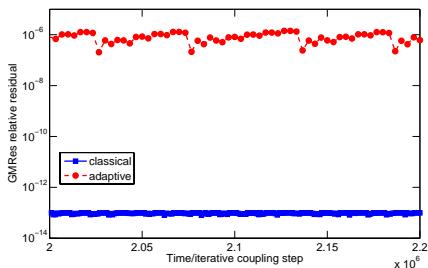


Estimators in function of
GMRes iterations

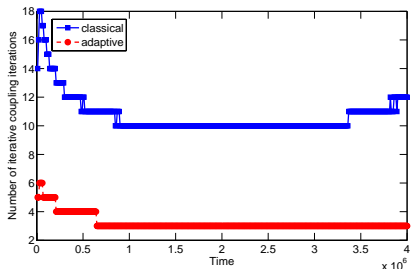


Estimators in function of
iterative coupling iterations

GMRes relative residual/iterative coupling iterations

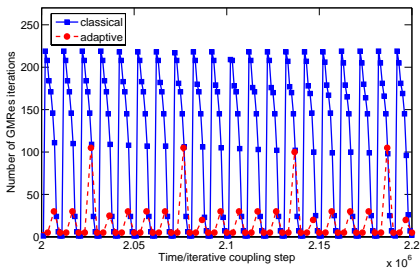


GMRes relative residual

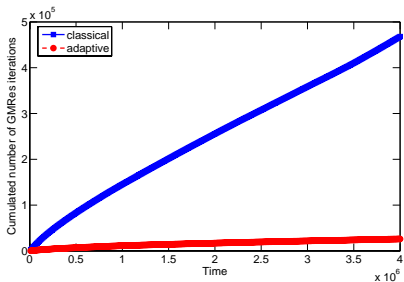


Iterative coupling iterations

GMRes iterations



Per time and iterative
coupling step



Cumulated

Outline

- 1 Introduction
- 2 Nonlinear diffusion
 - Quasi-linear elliptic problems
 - A guaranteed a posteriori error estimate
 - Stopping criteria and efficiency
 - Applications
 - Numerical results
- 3 The Stefan problem
 - Dual residual and energy norms
 - A posteriori error estimate and its efficiency
 - Numerical results
- 4 Two-phase immiscible incompressible flow
 - Weak solution
 - A posteriori error estimate and its efficiency
 - Applications and numerical results
- 5 Conclusions and future directions

Conclusions

Complete adaptivity

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

Future directions

- other coupled nonlinear systems
- convergence and optimality

Conclusions

Complete adaptivity

- only a **necessary number** of **algebraic solver iterations** on each linearization step
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- important **computational savings**
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Future directions

- other coupled nonlinear systems
- convergence and optimality

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Thank you for your attention!