Adaptive regularization, linearization, and algebraic solution in numerical discretizations

Martin Vohralík

INRIA Paris-Rocquencourt


Tokyo, November 9, 2012
I Nonlinear diffusion  Stefan problem  Two-phase flow  C

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
   - Regularization
   - A posteriori error estimate and its efficiency
   - Numerical results

4 Two-phase flow in porous media
   - A posteriori error estimate
   - Applications and numerical results

5 Conclusions and future directions

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5 Conclusions and future directions
Inexact Newton method

System of nonlinear algebraic equations
Nonlinear operator $A : \mathbb{R}^N \to \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

$$A(U) = F$$

Algorithm (Inexact linearization)

1. Choose initial vector $U^0$. Set $k := 1$.
2. $U^{k-1}$ ⇒ matrix $A^{k-1}$ and vector $F^{k-1}$: find $U^k$ s.t.
   
   $$A^{k-1}U^k \approx F^{k-1}.$$ 

3. 
   1. Set $U^{k,0} := U^{k-1}$ and $i := 1$.
   2. Do 1 algebraic solver step ⇒ $U^{k,i}$ s.t. ($R^{k,i}$ algebraic res.)
      
      $$A^{k-1}U^{k,i} = F^{k-1} - R^{k,i}.$$ 

   3. Convergence? OK ⇒ $U^k := U^{k,i}$. KO ⇒ $i := i + 1$, back to 3.2.

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4. Convergence? OK \( \Rightarrow \text{finish} \). KO \( \Rightarrow k := k + 1 \), back to 2.
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Approximate solution

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

Numerical method

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

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 $\|u - u^{k,i}_h\|$ on Newton step $k$ and algebraic solver step $i$, how is it distributed?
Context and questions

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Previous results

**Inexact Newton method**
- Eisenstat and Walker (1990’s)
- Moret (1989)

**Stopping criteria**
- engineering literature, since 1950’s
- Arioli (2000’s)

**A posteriori error estimates for 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, loc. cons. methods
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Quasi-linear elliptic problem

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  \[-\nabla \cdot \sigma(u, \nabla u) = f \quad \text{in } \Omega,\]
  \[u = 0 \quad \text{on } \partial \Omega\]

- Quasi-linear diffusion problem
  \[\sigma(u, \nabla u) = A(u) \nabla u\]

- Leray–Lions problem
  \[\sigma(u, \nabla u) = A(\nabla u) \nabla u\]

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

Example

- \(p\)-Laplacian: Leray–Lions setting with \(A(\nabla u) = |\nabla u|^{p-2} \nabla u\)

Nonlinear operator \(A : V := W^{1,p}_0(\Omega) \to V'\)

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

Weak formulation

Find \(u \in V\) such that

\[A(u) = f \quad \text{in } V'\]
Quasi-linear elliptic problem

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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 \( V \)

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})
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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} \right\}^{1/q}
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- there holds \( \mathcal{J}_u(u_h^{k,i}) = 0 \) if and only if \( u = u_h^{k,i} \)

- physical relevance: difference of the fluxes + nonconformity

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A posteriori error estimate

Assumption A (Total flux reconstruction)

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

$$\nabla \cdot t_h^{k,i} = f - \rho_h^{k,i}.$$ 

Theorem (A posteriori error estimate)

Let

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

Then there holds

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

where $\eta_h^{k,i}$ is fully computable from $u_h^{k,i}, t_h^{k,i},$ and $\rho_h^{k,i}$.
A posteriori error estimate

Assumption A (Total flux reconstruction)

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

$$\nabla \cdot t_h^{k,i} = f - \rho_h^{k,i}.$$ 

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

$$J_u(u_h^{k,i}) \leq \eta_h^{k,i},$$

where $\eta_h^{k,i}$ is fully computable from $u_h^{k,i}$, $t_h^{k,i}$, and $\rho_h^{k,i}$. 
A posteriori error estimate

Assumption A (Total flux reconstruction)

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

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Theorem (A posteriori error estimate)

Let

- $u \in V$ be the weak solution,
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- Assumption A hold.

Then there holds

$$\mathcal{J}_u(u^{k,i}_h) \leq \tilde{\eta}^{k,i}_h,$$

where $\tilde{\eta}^{k,i}_h$ is fully computable from $u^{k,i}_h$, $\mathbf{t}^{k,i}_h$, and $\rho^{k,i}_h$.
Distinguishing error components

Assumption B (Discretization, linearization, and algebraic errors)

There exist fluxes $d_{h}^{k,i}, l_{h}^{k,i}, a_{h}^{k,i} \in [L^q(\Omega)]^d$ such that

(i) $d_{h}^{k,i} + l_{h}^{k,i} + a_{h}^{k,i} = t_{h}^{k,i}$;

(ii) as the linear solver converges, $\|a_{h}^{k,i}\|_q \to 0$;

(iii) as the nonlinear solver converges, $\|l_{h}^{k,i}\|_q \to 0$.

Comments

- $d_{h}^{k,i}$: discretization flux reconstruction
- $l_{h}^{k,i}$: linearization error flux reconstruction
- $a_{h}^{k,i}$: algebraic error flux reconstruction
Distinguishing error components

Assumption B (Discretization, linearization, and algebraic errors)

There exist fluxes $d_h^{k,i}, l_h^{k,i}, a_h^{k,i} \in [L^q(\Omega)]^d$ such that

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- $d_h^{k,i}$: discretization flux reconstruction
- $l_h^{k,i}$: linearization error flux reconstruction
- $a_h^{k,i}$: algebraic error flux reconstruction
Theorem (Estimate distinguishing different error components)

Let
- \( u \in V \) be the weak solution,
- \( u_{k,i}^h \in V(T_h) \) be arbitrary,
- Assumptions A and B hold.

Then there holds

\[ J_u(u_{k,i}^h) \leq \eta_{k,i}^h := \eta_{\text{disc}}^k + \eta_{\text{lin}}^k + \eta_{\text{alg}}^k + \eta_{\text{rem}}^k. \]
Theorem (Estimate distinguishing different error components)

Let
- \( u \in V \) be the weak solution,
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\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}.
\]
Estimators

- **discretization estimator**

\[ \eta_{\text{disc},K}^{k,i} := 2^{1/p} \left( \| \sigma(u_h^{k,i}, \nabla u_h^{k,i}) + d_h^{k,i} \|_{q,K} + \left\{ \sum_{e \in E_K} h_e^{1-q} \| [u_h^{k,i}]_{q,e} \|_{q,e} \right\}^{1/q} \right) \]

- **linearization estimator**

\[ \eta_{\text{lin},K}^{k,i} := \| l_h^{k,i} \|_{q,K} \]

- **algebraic estimator**

\[ \eta_{\text{alg},K}^{k,i} := \| a_h^{k,i} \|_{q,K} \]

- **algebraic remainder estimator**

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

- \[ \eta^{k,i} := \left\{ \sum_{K \in T_h} (\eta_{\cdot, K}^{k,i})^q \right\}^{1/q} \]
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
   - Regularization
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4. Two-phase flow in porous media
   - A posteriori error estimate
   - Applications and numerical results

5. Conclusions and future directions
Stopping criteria

Global stopping criteria

- stop whenever:
  \[
  \eta_{alg, i}^k \leq \gamma_{alg, max} \max\{\eta_{disc, i}^k, \eta_{lin, i}^k\},
  \eta_{lin, i}^k \leq \gamma_{lin, disc} \eta_{disc, i}^k
  \]

- \(\gamma_{alg, max}, \gamma_{lin} \approx 0.1\)

Local stopping criteria

- stop whenever:
  \[
  \eta_{alg, K, i}^k \leq \gamma_{alg, K, max} \max\{\eta_{disc, K, i}^k, \eta_{lin, K, i}^k\}, \quad \forall K \in T_h,
  \eta_{lin, K, i}^k \leq \gamma_{lin, K} \eta_{disc, K, i}^k \quad \forall K \in T_h
  \]

- \(\gamma_{alg, K, max}, \gamma_{lin, K} \approx 0.1\)
Stopping criteria

Global stopping criteria

- stop whenever:
  \[ \eta_{alg}^{k,i} \leq \gamma_{alg} \max\{ \eta_{disc}^{k,i}, \eta_{lin}^{k,i} \}, \]
  \[ \eta_{lin}^{k,i} \leq \gamma_{lin} \eta_{disc}^{k,i} \]

- \( \gamma_{alg}, \gamma_{lin} \approx 0.1 \)

Local stopping criteria

- stop whenever:
  \[ \eta_{alg,K}^{k,i} \leq \gamma_{alg,K} \max\{ \eta_{disc,K}^{k,i}, \eta_{lin,K}^{k,i} \} \quad \forall K \in \mathcal{T}_h, \]
  \[ \eta_{lin,K}^{k,i} \leq \gamma_{lin,K} \eta_{disc,K}^{k,i} \quad \forall K \in \mathcal{T}_h \]

- \( \gamma_{alg,K}, \gamma_{lin,K} \approx 0.1 \)
Assumption C (Approximation property)

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

$$\| \bar{\sigma}^{k,i}_h + d^{k,i}_h \|_{q,K} \lesssim \eta^{k,i}_{\#}, \mathcal{T}_K + \eta^{k,i}_{\text{osc}, \mathcal{T}_K},$$

where

$$\eta^{k,i}_{\#}, \mathcal{T}_K := \left\{ \sum_{K' \in \mathcal{T}_K} h^{q}_{K'} \| f_h + \nabla \cdot \sigma^{k,i}_h \|_{q,K'} + \sum_{e \in e_{\text{int}}^h} h_{e} \| [\sigma^{k,i}_h \cdot n_e] \|_{q,e} \right\}^{-\frac{1}{q}} + \sum_{e \in e_{\text{e}}^h} h_{e}^{1-q} \| [u^{k,i}_h] \|_{q,e}.$$
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,

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

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.
Global efficiency

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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,

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- robustness with respect to the nonlinearity thanks to the choice of the dual norm as error measure
Theorem (Local efficiency)

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

\[
\eta_{\text{disc},K}^{k,i} + \eta_{\text{lin},K}^{k,i} + \eta_{\text{alg},K}^{k,i} + \eta_{\text{rem},K}^{k,i} \lesssim \mathcal{J}_{u,\mathcal{K}}^{\text{up}}(u_h^{k,i})
\]

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

- robustness and **local efficiency** for an upper bound on the dual norm
Theorem (Local efficiency)

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

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

- robustness and local efficiency for an upper bound on the dual norm
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5. Conclusions and future directions
Construction of $a_h^{k,i}$ and $ρ_h^{k,i}$

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

$$ musica^{k U^{k,i}} = F^k - R^{k,i}.$$ 

Do $ν$ additional steps of the algebraic solver, yielding

$$ musica^{k U^{k,i+ν}} = F^k - R^{k,i+ν}.$$ 

Construct the function $ρ_h^{k,i}$ from the algebraic residual vector $R_h^{k,i+ν}$ (lifting into appropriate discrete space).

Suppose we can obtain discretization and linearization flux reconstructions $d_h^{k,i}$, $l_h^{k,i}$ on each algebraic step. Then set

$$ a_h^{k,i} := (d_h^{k,i+ν} + l_h^{k,i+ν}) - (d_h^{k,i} + l_h^{k,i}).$$

Independent of the algebraic solver.
Construction of $a_{h}^{k,i}$ and $\rho_{h}^{k,i}$

- On linearization step $k$ and algebraic step $i$, we have
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Algebraic error flux and algebraic remainder

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- Independent of the algebraic solver.
Example: nonconforming finite elements for the $p$-Laplacian

Discretization

Find $u_h \in V_h$ such that

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

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

$A(U) = F$
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- \( V_h \) the Crouzeix–Raviart space
- leads to the system of nonlinear algebraic equations

\[
\mathcal{A}(U) = F
\]
Linearization

Find $u_h^k \in V_h$ such that

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

- $u_h^0 \in V_h$ yields the initial vector $U^0$
- fixed-point linearization
  
  $\sigma^{k-1}(\xi) := |\nabla u_h^{k-1}|^{p-2} \xi$

- Newton linearization
  
  $\sigma^{k-1}(\xi) := |\nabla u_h^{k-1}|^{p-2} \xi + (p - 2)|\nabla u_h^{k-1}|^{p-4} 
  (\nabla u_h^{k-1} \otimes \nabla u_h^{k-1})(\xi - \nabla u_h^{k-1})$

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Linearization

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$$A^k U^k = F^k$$
Algebraic solution

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

$$(\sigma^{k-1}(\nabla u_h^k, i), \nabla \psi_e) = (f, \psi_e) - R_{e}^{k, i} \quad \forall e \in E_{h}^{\text{int}}.$$ 

- algebraic residual vector $R_{e}^{k, i} = \{R_{e}^{k, i}\}_{e \in E_{h}^{\text{int}}}$
- discrete system

$$A^k U^k = F^k - R^{k, i}$$
Algebraic solution

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

\[
(\sigma^{k-1}(\nabla u_h^{k,i}), \nabla \psi_e) = (f, \psi_e) - R^{k,i}_e \quad \forall e \in \mathcal{E}_h^{\text{int}}.
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- **algebraic residual vector** \( R^{k,i}_e = \{ R^{k,i}_e \}_{e \in \mathcal{E}_h^{\text{int}}} \)
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\[
\mathbb{A}^k U^k = F^k - R^{k,i}_e
\]
Definition (Construction of \(d^{k,i}_h\))

For all \(K \in \mathcal{T}_h\),

\[
d^{k,i}_h|_K := -\sigma(\nabla u^{k,i}_h)|_K + \frac{f|_K}{d}(x - x_K) - \sum_{e \in \mathcal{E}_h} \frac{\bar{R}^{k,i}_e}{d |D_e|} (x - x_K)|_{K_e},
\]

where \(\bar{R}^{k,i}_e := (f, \psi_e) - (\sigma(\nabla u^{k,i}_h), \nabla \psi_e)\) \(\forall e \in \mathcal{E}^{\text{int}}_h\).

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\]
Flux reconstructions

Definition (Construction of $d_h^{k,i}$)

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Adaptive regularization, linearization, and algebraic solution
Verification of the assumptions

Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

- \( \| a^{k,i}_h \|_{q,K} \to 0 \) as the linear solver converges by definition.
- \( \| l^{k,i}_h \|_{q,K} \to 0 \) as the nonlinear solver converges by the construction of \( l^{k,i}_h \).

Lemma (Assumption C)

Assumption C holds.

Comments

- \( d^{k,i}_h \) close to \( \sigma(\nabla u^{k,i}_h) \)
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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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Adaptive regularization, linearization, and algebraic solution

Numerical experiment I

Model problem

- \( p \)-Laplacian

\[ \nabla \cdot (|\nabla u|^{p-2} \nabla u) = f \quad \text{in } \Omega, \]

\[ u = u_0 \quad \text{on } \partial \Omega \]

- 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 value \( p = 10 \)

- nonconforming finite elements

M. Vohralík  Adaptive regularization, linearization, and algebraic solution
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
Error and estimators, $p = 10$

Newton

inexact Newton

ad. inexact Newton
Newton and algebraic iterations, $p = 10$

- Newton it. / refinement
- alg. it. / Newton step
- alg. it. / refinement

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Adaptive regularization, linearization, and algebraic solution
Model problem

- $p$-Laplacian

\[ \nabla \cdot (|\nabla u|^{p-2} \nabla u) = f \quad \text{in } \Omega, \]
\[ u = u_0 \quad \text{on } \partial \Omega \]

- 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**
- Left graph: Plot showing energy error against the number of faces.
- The graph compares energy error uniform and energy error adaptive.

**Overall performance**
- Right graph: Plot showing the total number of algebraic solver iterations against refinement level.
- The graph compares uniform and adaptive methods.

M. Vohralík
Adaptive regularization, linearization, and algebraic solution
Outline

1. Introduction

2. Nonlinear diffusion
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   - A guaranteed a posteriori error estimate
   - Stopping criteria and efficiency
   - Applications
   - Numerical results

3. The Stefan problem
   - Regularization
   - A posteriori error estimate and its efficiency
   - Numerical results

4. Two-phase flow in porous media
   - A posteriori error estimate
   - Applications and numerical results

5. Conclusions and future directions
The Stefan problem

\[\partial_t u - \Delta \beta(u) = f \quad \text{in } \Omega \times (0, T),\]
\[u(\cdot, 0) = u_0 \quad \text{in } \Omega,\]
\[\beta(u) = 0 \quad \text{on } \partial \Omega \times (0, T)\]

Nomenclature

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

\[ \partial_t u - \Delta \beta(u) = f \quad \text{in } \Omega \times (0, T), \]
\[ u(\cdot, 0) = u_0 \quad \text{in } \Omega, \]
\[ \beta(u) = 0 \quad \text{on } \partial \Omega \times (0, T) \]

Nomenclature

- \( u \) enthalpy, \( \beta(u) \) temperature
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- phase change, degenerate parabolic problem
- \( u_0 \in L^2(\Omega), f \in L^2(0, T; L^2(\Omega)) \)
Residual and its dual norm

Functional spaces

\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

Weak formulation

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

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

\[ \langle \partial_t u, \varphi \rangle(t) + (\nabla \beta(u), \nabla \varphi)(t) = (f, \varphi)(t) \quad \forall \varphi \in H^1_0(\Omega) \quad \text{a.e.} \ t \in (0, T) \]

Residual for \( u_{h^T} \in Z \) such that \( \beta(u_{h^T}) \in X \)

\[ \langle \mathcal{R}(u_{h^T}), \varphi \rangle_{X', X} = \int_0^T \left\{ \langle \partial_t (u - u_{h^T}), \varphi \rangle + (\nabla \beta(u) - \nabla \beta(u_{h^T}), \nabla \varphi) \right\}(t) \, dt, \quad \varphi \in X \]

Dual norm of the residual

\[ \| \mathcal{R}(u_{h^T}) \|_{X'} := \sup_{\varphi \in X, \| \varphi \|_X = 1} \langle \mathcal{R}(u_{h^T}), \varphi \rangle_{X', X} \]
Residual and its dual norm

Functional spaces

\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

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\[ u(\cdot, 0) = u_0 \quad \text{in } \Omega \]
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Residual for \( u_{hT} \in Z \) such that \( \beta(u_{hT}) \in X \)

\[ \langle \mathcal{R}(u_{hT}), \varphi \rangle_{X', X} = \int_0^T \left\{ \langle \partial_t (u - u_{hT}), \varphi \rangle + (\nabla \beta(u) - \nabla \beta(u_{hT}), \nabla \varphi) \right\}(t) \, dt, \]

\[ \varphi \in X \]

Dual norm of the residual

\[ \| \mathcal{R}(u_{hT}) \|_{X'} : = \sup_{\varphi \in X, \| \varphi \|_X = 1} \langle \mathcal{R}(u_{hT}), \varphi \rangle_{X', X} \]
Residual and its dual norm

Functional spaces
\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

Weak formulation
\[ u \in Z \quad \text{with} \quad \beta(u) \in X \]
\[ u(\cdot, 0) = u_0 \quad \text{in} \quad \Omega \]
\[ \langle \partial_t u, \varphi \rangle(t) + (\nabla \beta(u), \nabla \varphi)(t) = (f, \varphi)(t) \quad \forall \varphi \in H^1_0(\Omega) \quad \text{a.e.} \quad t \in (0, T) \]

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
\[ X := L^2(0, T; H^1_0(\Omega)), \quad Z := H^1(0, T; H^{-1}(\Omega)) \]

Weak formulation
\[ u \in Z \quad \text{with} \quad \beta(u) \in X \]
\[ u(\cdot, 0) = u_0 \quad \text{in} \quad \Omega \]
\[ \langle \partial_t u, \varphi \rangle(t) + (\nabla \beta(u), \nabla \varphi)(t) = (f, \varphi)(t) \quad \forall \varphi \in H^1_0(\Omega) \quad \text{a.e.} \ t \in (0, T) \]

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
\[ \| \mathcal{R}(u_{h\tau}) \|_{X'} := \sup_{\varphi \in X, \| \varphi \|_X = 1} \langle \mathcal{R}(u_{h\tau}), \varphi \rangle_{X', X} \]
Regularization with a parameter $\epsilon$

\[ \beta(u), \beta^{\epsilon}(u) \]
Practice: questions

Discretization

- ...

Question (Stopping and balancing criteria)

- What is a good choice of the regularization parameter $\epsilon$?
- time step?
- space mesh?

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

Question (Error)

- How big is the error $\| u|_{I_n} - u_{ht}^{n,\epsilon,k,i} \|$ on time step $n$, space mesh $T_h^n$, for the regularization parameter $\epsilon$, 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

- ...

#### Question (Stopping and balancing criteria)

- **What is a good choice of the**
  - regularization parameter $\epsilon$?
  - time step?
  - space mesh?

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

#### Question (Error)

- **How big is the error** $\| u^n_h - u_{h_T}^{n,\epsilon,k,i} \|$ **on time step** $n$, **space mesh** $T_h^n$, **for the regularization parameter** $\epsilon$, **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

...)

Question (Stopping and balancing criteria)

- **What is a good choice of the**
  - regularization parameter $\epsilon$?
  - time step?
  - space mesh?

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

Question (Error)

- **How big is the error** $\| u^n - u_h^{n,\epsilon,k,i} \|$ **on time step** $n$, **space mesh** $T_h^n$, **for the regularization parameter** $\epsilon$, **Newton step** $k$, **and algebraic solver step** $i$? **How big are the individual components? How is error distributed in time and space?**
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Theorem (Estimate and its efficiency)

There holds

\[ \| \mathcal{R}(u_{h\tau}) \|_{X'} + \| u_0 - u_{h\tau}(0) \|_{H^{-1}(\Omega)} \]

\[ \leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K \in \mathcal{T}_h^n} (\eta_{R,K}^n + \eta_{F,K}^n)^2 \right\}^{\frac{1}{2}} + \eta_{IC} \]

\[ \lesssim \| \mathcal{R}(u_{h\tau}) \|_{X'} + \| u_0 - u_{h\tau}(0) \|_{H^{-1}(\Omega)} , \]

with

\[ \eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{h\tau} - \nabla \cdot t^n_h \|_K , \]

\[ \eta_{F,K}^n(t) := \| \nabla \beta(u_{h\tau}(t)) + t^n_h \|_K , \]

\[ \eta_{IC} := \| u_0 - u_{h\tau}(0) \|_{H^{-1}(\Omega)} . \]

Theorem (An estimate distinguishing the error components)

For time \( n \), linearization \( k \), and regularization \( \epsilon \), there holds

\[ \| \mathcal{R}(u^{n,\epsilon,k}_{h\tau}) \|_{X', I_n} \leq \eta_{sp}^{n,\epsilon,k} + \eta_{tm}^{n,\epsilon,k} + \eta_{lin}^{n,\epsilon,k} + \eta_{reg}^{n,\epsilon,k} . \]
A posteriori estimate and its efficiency

**Theorem (Estimate and its efficiency)**

There holds

\[
\| R(u_{h_T}) \|_{X'} + \| u_0 - u_{h_T}(0) \|_{H^{-1}(\Omega)} \leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K \in T_h^n} (\eta_{R,K}^n + \eta_{F,K}^n)^2 \right\}^{1/2} + \eta_{IC}
\]

with

\[
\eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{h_T} - \nabla \cdot t^n_h \|_K,
\]

\[
\eta_{F,K}^n(t) := \| \nabla \beta(u_{h_T}(t)) + t^n_h \|_K,
\]

\[
\eta_{IC} := \| u_0 - u_{h_T}(0) \|_{H^{-1}(\Omega)}.
\]

**Theorem (An estimate distinguishing the error components)**

For time \( n \), linearization \( k \), and regularization \( \epsilon \), there holds

\[
\| R(u_{h_T}^{n,\epsilon,k}) \|_{X',I_n} \leq \eta_{sp}^{n,\epsilon,k} + \eta_{tm}^{n,\epsilon,k} + \eta_{lin}^{n,\epsilon,k} + \eta_{reg}^{n,\epsilon,k}.
\]
Theorem (A posteriori estimate and its efficiency)

There holds

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

\[ \lesssim \| \mathcal{R}(u_{h\tau}) \|_{X'} + \| u_0 - u_{h\tau}(0) \|_{H^{-1}(\Omega)}, \]

with

\[ \eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{h\tau} - \nabla \cdot t^n_h \|_K, \]

\[ \eta_{F,K}^n(t) := \| \nabla \beta(u_{h\tau}(t)) + t^n_h \|_K, \]

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Theorem (An estimate distinguishing the error components)

For time \( n \), linearization \( k \), and regularization \( \epsilon \), there holds

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Theorem (Estimate and its efficiency)

There holds

\[
\| \mathcal{R}(u_{hT}) \|_{X'} + \| u_0 - u_{hT}(0) \|_{H^{-1}(\Omega)} \\
\leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K \in T_h^n} (\eta_{R,K}^n + \eta_{F,K}^n)^2 \right\}^{1/2} + \eta_{IC}
\]

with

\[
\eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{hT} - \nabla \cdot t_h^n \|_K,
\]

\[
\eta_{F,K}^n(t) := \| \nabla \beta(u_{hT}(t)) + t_h^n \|_K,
\]

\[
\eta_{IC} := \| u_0 - u_{hT}(0) \|_{H^{-1}(\Omega)}.
\]

Theorem (An estimate distinguishing the error components)

For time \( n \), linearization \( k \), and regularization \( \epsilon \), there holds

\[
\| \mathcal{R}(u_{hT}^{n, \epsilon, k}) \|_{X', I_n} \leq \eta_{sp}^{n, \epsilon, k} + \eta_{tm}^{n, \epsilon, k} + \eta_{lin}^{n, \epsilon, k} + \eta_{reg}^{n, \epsilon, k}.
\]
A posteriori estimate and its efficiency

Theorem (Estimate and its efficiency)

There holds

\[
\| \mathcal{R}(u_{h,T}) \|_{X} + \| u_0 - u_{h,T}(0) \|_{H^{-1}(\Omega)} \leq \left\{ \sum_{n=1}^{N} \int_{I_n} \sum_{K \in T_h^n} \left( \eta_{R,K}^n + \eta_{F,K}^n \right)^2 \right\}^{\frac{1}{2}} + \eta_{IC}
\]

\[
\lesssim \| \mathcal{R}(u_{h,T}) \|_{X} + \| u_0 - u_{h,T}(0) \|_{H^{-1}(\Omega)},
\]

with

\[ \eta_{R,K}^n := C_{P,K} h_K \| f^n - \partial_t u_{h,T} - \nabla \cdot t_h^n \|_{K}, \]

\[ \eta_{F,K}(t) := \| \nabla \beta(u_{h,T}(t)) + t_h^n \|_{K}, \]

\[ \eta_{IC} := \| u_0 - u_{h,T}(0) \|_{H^{-1}(\Omega)}. \]

Theorem (An estimate distinguishing the error components)

For time \( n \), linearization \( k \), and regularization \( \epsilon \), there holds

\[
\| \mathcal{R}(u_{h,T}^{n,\epsilon,k}) \|_{X}, I_n \leq \eta_{sp}^{n,\epsilon,k} + \eta_{tm}^{n,\epsilon,k} + \eta_{lin}^{n,\epsilon,k} + \eta_{reg}^{n,\epsilon,k}.
\]
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Adaptive regularization, linearization, and algebraic solution
Linearization stopping criterion

\[ \eta_{lin}^{n,\varepsilon,k} \leq \gamma_{lin}(\eta_{sp}^{n,\varepsilon,k} + \eta_{tm}^{n,\varepsilon,k} + \eta_{reg}^{n,\varepsilon,k}) \]

Number of Newton iterations

- Space error
- Time error
- Regul. error
- Lin. error
Regularization stopping criterion

\[ \eta_{n,\epsilon,k} \leq \gamma_{\text{reg}} \left( \eta_{n,\epsilon,k}^{\text{sp}} + \eta_{n,\epsilon,k}^{\text{tm}} \right) \]
Equilibrating time and space errors

\[ \gamma_{\min} \eta_{sp}^{\epsilon,n,k} \leq \eta_{tm}^{\epsilon,n,k} \leq \gamma_{\max} \eta_{sp}^{\epsilon,n,k} \]

- Total number of space-time unknowns
- Space error
- Time error

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Adaptive regularization, linearization, and algebraic solution
Error and estimate

![Graph showing error and estimate](image)

- Error adapt.
- Error unif.

Total number of space-time unknowns

Error

- $10^{-0.4}$
- $10^{-0.6}$
- $10^{-0.8}$
Effectivity indices

![Graph showing effectivity indices versus total number of space-time unknowns. The graph includes two lines: one for 'Eff. ind. adapt.' and another for 'Eff. ind. unif.' The y-axis represents the effectivity index ranging from 10^4 to 10^7. The x-axis represents the total number of space-time unknowns, ranging from 10^4 to 10^7. The graph shows a decreasing trend as the total number of space-time unknowns increases.]

- **Eff. ind. adapt.**
- **Eff. ind. unif.**

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Adaptive regularization, linearization, and algebraic solution
Actual and estimated error distribution

Adaptive regularization, linearization, and algebraic solution
Computational efficiency

Figure: Number of cumulated Newton iterations vs. error estimate.
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Two-phase flow in porous media

\[
\partial_t (\phi s_\alpha) + \nabla \cdot u_\alpha = q_\alpha, \quad \alpha \in \{n, w\},
\]

\[
-k_{r,\alpha}(s_w) \frac{K(\nabla p_\alpha + \rho_\alpha g \nabla z)}{\mu_\alpha} = u_\alpha, \quad \alpha \in \{n, w\},
\]

\[s_n + s_w = 1,\]

\[p_n - p_w = p_c(s_w).\]

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–parabolic degenerate type
- dominant advection
Two-phase flow in porous media

\[ \partial_t (\phi s_\alpha) + \nabla \cdot u_\alpha = q_\alpha, \quad \alpha \in \{n, w\}, \]

\[ - \frac{k_{r,\alpha}(s_w)}{\mu_\alpha} K (\nabla p_\alpha + \rho_\alpha g \nabla z) = u_\alpha, \quad \alpha \in \{n, w\}, \]

\[ s_n + s_w = 1, \]

\[ \rho_n - \rho_w = p_c(s_w). \]

Mathematical issues

- coupled system
- unsteady, nonlinear
- elliptic–parabolic degenerate type
- dominant advection
I Nonlinear diffusion  Stefan problem  Two-phase flow

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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 $(s_{\alpha, h_T}^{k,i}, p_{\alpha, h_T}^{k,i})$. Then

$$|||(s_{\alpha} - s_{\alpha, h_T}^{k,i}, p_{\alpha} - p_{\alpha, h_T}^{k,i})|||_n \leq \eta_{sp, \alpha}^{n,k,i} + \eta_{tm, \alpha}^{n,k,i} + \eta_{lin, \alpha}^{n,k,i} + \eta_{alg, \alpha}^{n,k,i}.$$ 

Error components

- $\eta_{sp, \alpha}^{n,k,i}$: spatial discretization
- $\eta_{tm, \alpha}^{n,k,i}$: temporal discretization
- $\eta_{lin, \alpha}^{n,k,i}$: linearization
- $\eta_{alg, \alpha}^{n,k,i}$: algebraic solver
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 \((s_{\alpha, h^\tau}^k, p_{\alpha, h^\tau}^k)\). Then

\[
\| | (s_{\alpha} - s_{\alpha, h^\tau}^k, p_{\alpha} - p_{\alpha, h^\tau}^k) \| |_{n} \leq \eta_{\text{sp}, \alpha}^{n,k,i} + \eta_{\text{tm}, \alpha}^{n,k,i} + \eta_{\text{lin}, \alpha}^{n,k,i} + \eta_{\text{alg}, \alpha}^{n,k,i}.
\]

Error components
- \( \eta_{\text{sp}, \alpha}^{n,k,i} \): spatial discretization
- \( \eta_{\text{tm}, \alpha}^{n,k,i} \): temporal discretization
- \( \eta_{\text{lin}, \alpha}^{n,k,i} \): linearization
- \( \eta_{\text{alg}, \alpha}^{n,k,i} \): algebraic solver
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5. Conclusions and future directions
Cell-centered finite volume scheme

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

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

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

where the fluxes are given by

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

$$
F_{n,e_{KK'}}(\mathbf{s}^n_{w,h}, \mathbf{\bar{p}}^n_{w,h}) := -\frac{\eta_{r,n}(\mathbf{s}^n_{w,K}) + \eta_{r,n}(\mathbf{s}^n_{w,K'})}{2} |K| \left( \mathbf{\bar{p}}^n_{w,K'} + \pi(\mathbf{s}^n_{w,K'}) - (\mathbf{\bar{p}}^n_{n,K} + \pi(\mathbf{s}^n_{n,K})) \right) \frac{1}{|\mathbf{x}_K - \mathbf{x}_{K'}|} |e_{KK'}|.
$$
Cell-centered finite volume scheme

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

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

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

where the fluxes are given by

\[
F_{w,e_{KK}'}(s^{n}_{w,h}, \bar{p}^{n}_{w,h}) := -\frac{\eta_{r,w}(s^{n}_{w,K}) + \eta_{r,w}(s^{n}_{w,K'})}{2} |K| \frac{\bar{p}^{n}_{w,K'} - \bar{p}^{n}_{w,K}}{|x_K - x_{K'}|} |e_{KK}'|,
\]

\[
F_{n,e_{KK}'}(s^{n}_{w,h}, \bar{p}^{n}_{w,h}) := -\frac{\eta_{r,n}(s^{n}_{w,K}) + \eta_{r,n}(s^{n}_{w,K'})}{2} |K| \times \frac{\bar{p}^{n}_{w,K'} + \pi(s^{n}_{w,K'}) - (\bar{p}^{n}_{n,K} + \pi(s^{n}_{n,K}))}{|x_K - x_{K'}|} |e_{KK}'|.
\]
Nonlinear diffusion Stefan problem Two-phase flow

A posteriori error estimate Applications and numerical results

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

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

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

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

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

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

where the linearized fluxes are given by

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

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

\[
(d_{\alpha,h}^{n,k,i} \cdot n_K, 1)_{e_{KK'}} := F_{\alpha,e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}),
\]

\[
((d_{\alpha,h}^{n,k,i} + l_{\alpha,h}^{n,k,i}) \cdot n_K, 1)_{e_{KK'}} := F^{k-1}_{\alpha,e_{KK'}}(s_{w,h}^{n,k,i}, \bar{p}_{w,h}^{n,k,i}),
\]

\[
a_{\alpha,h}^{n,k,i} := d_{\alpha,h}^{n,k,i+\nu} + l_{\alpha,h}^{n,k,i+\nu} - (d_{\alpha,h}^{n,k,i} + l_{\alpha,h}^{n,k,i})
\]
I  Nonlinear diffusion  Stefan problem  Two-phase flow  C  A posteriori error estimate  Applications and numerical results

Water saturation estimators evolution

M. Vohralík  Adaptive regularization, linearization, and algebraic solution
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

M. Vohralík
Adaptive regularization, linearization, and algebraic solution
GMRes iterations

Per time and Newton 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
   - Regularization
   - A posteriori error estimate and its efficiency
   - Numerical results
4. Two-phase flow in porous media
   - A posteriori error estimate
   - 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
- 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
- only a **necessary number** of **linearization iterations**
- **optimal** choice of the **regularization parameter**
- space-time mesh adaptivity
- important **computational savings**
- guaranteed and robust upper bound via **a posteriori error estimates**

Future directions

- other coupled nonlinear systems
- convergence and optimality


VOHRALÍK M., WHEELER M. F., A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows, HAL Preprint 00633594.


Thank you for your attention!