Adaptive inexact Newton methods and adaptive regularization and space–time discretization for unsteady nonlinear problems

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Full adaptivity for unsteady nonlinear problems

Real (porous media) flows

- system of PDEs
- nonlinear (degenerate)
- unsteady
- $\Rightarrow$ difficult numerical approximation, large troublesome **systems** of **nonlinear algebraic equations**

Goals of this work

- derive fully computable a posteriori **error upper bounds**
- distinguish different **error components**

Full adaptivity

- time step choice & mesh adaptivity
- **stopping criteria** for **regularization** and **linear** and **nonlinear** solvers

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Previous results – a posteriori error estimates

Nonlinear steady problems

- Ladevèze (since 1990's), guaranteed upper bound
- Verfürth (1994), residual estimates
- Carstensen and Klose (2003), *p*-Laplacian
- 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

Nonlinear unsteady problems

- Verfürth (1998), framework for energy norm control
- Ohlberger (2001), non energy-norm estimates

Degenerate parabolic problems

- Nochetto, Schmidt, Verdi (2000), Stefan problem
- Dolejší, Ern, Vohralík (2013), ADR, Richards, robustness in a space–time dual mesh-dependent norm

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Adaptive inexact Newton method

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- Hackbusch and Reusken (1989), damping and multigrid
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Model errors

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Outline

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2. Adaptive inexact Newton method
   - A posteriori error estimate and its efficiency
   - Applications
   - Numerical results
3. The Stefan problem
   - Dual norm a posteriori estimate and adaptivity
   - Efficiency
   - Energy error a posteriori estimate
   - Numerical results
4. Conclusions and future directions

Inexact iterative linearization

System of nonlinear algebraic equations

Nonlinear operator $\mathcal{A}: \mathbb{R}^N \to \mathbb{R}^N$, vector $F \in \mathbb{R}^N$: find $U \in \mathbb{R}^N$ s.t.

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

Algorithm (Inexact iterative linearization)

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

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

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

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

   3. *Convergence? OK* $\Rightarrow U^k := U^{k,i}$. *KO* $\Rightarrow i := i + 1$, *back to 3.2.*
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Context and questions

Approximate solution

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

Numerical method

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

Partial differential equation

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

Question (Stopping criteria)

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

Question (Error)

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

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Model steady problem, discretization

Quasi-linear elliptic problem

$$-\nabla\cdot\boldsymbol{\sigma}(u,\nabla u) = f \qquad \text{in } \Omega,$$
$$u = 0 \qquad \text{on } \partial\Omega$$

- $p > 1$, $q := \frac{p}{p-1}$, $f \in L^q(\Omega)$
- example: p-Laplacian with $\boldsymbol{\sigma}(u,\nabla u) = |\nabla u|^{p-2}\nabla u$
- f piecewise polynomial for simplicity
- weak solution: $u \in V := W_0^{1,p}(\Omega)$ such that

$$(\boldsymbol{\sigma}(u,\nabla u),\nabla v) = (f,v) \qquad \forall v \in V$$

Numerical approximation

- (shape-regular) mesh $\mathcal{T}_h$, linearization step k, algebraic step i
- $u_h^{k,i} \in V(\mathcal{T}_h)$ piecewise polynomial (discontinuous), $V(\mathcal{T}_h) \not\subset V$

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Abstract assumptions

Assumption A (Total flux reconstruction)

There exists $\mathbf{t}_h^{k,i} \in \mathbf{H}^q(\mathrm{div}, \Omega)$ *and* $\rho_h^{k,i} \in L^q(\Omega)$ *such that*

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

Assumption B (Discretization, linearization, and alg. fluxes)

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) $\mathbf{t}_h^{k,i} = \mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i} + \mathbf{a}_h^{k,i}$;

(ii) *as the linear solver converges,* $\|\mathbf{a}_h^{k,i}\|_q \to 0$;

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Assumption C (Approximation property)

$$\|\boldsymbol{\sigma}(u_h^{k,i}, \nabla u_h^{k,i}) + \mathbf{d}_h^{k,i}\|_q \leq C \text{ (residual estimator).}$$

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Estimate distinguishing error components

Theorem (Estimate distinguishing different error components)

Let

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

Then there holds

$$\mathcal{J}_u(u_h^{k,i}) \leq \eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i}.$$

Moreover, under Assumption C and under appropriate stopping criteria,

$$\eta_{\mathrm{disc}}^{k,i} + \eta_{\mathrm{lin}}^{k,i} + \eta_{\mathrm{alg}}^{k,i} + \eta_{\mathrm{rem}}^{k,i} \leq C\mathcal{J}_u(u_h^{k,i}),$$

up to quadrature errors.

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Estimators

- *discretization* estimator

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

- *linearization* estimator

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

- *algebraic* estimator

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

- *algebraic remainder estimator*

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

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

Outline

Nonconforming finite elements for the p-Laplacian

Discretization

Find $u_h \in V_h$ such that

$$(\boldsymbol{\sigma}(\nabla u_h), \nabla v_h) = (f_h, v_h) \qquad \forall v_h \in V_h.$$

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

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

Nonconforming finite elements for the p-Laplacian

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Linearization

Linearization

Find $u_h^k \in V_h$ such that

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

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

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

- Newton linearization

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

- leads to the system of linear algebraic equations

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

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Linearization

Find $u_h^k \in V_h$ such that

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

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

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

- Newton linearization

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

- leads to the system of linear algebraic equations

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

Algebraic solution

Algebraic solution

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

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

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

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

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Flux reconstructions

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

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

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

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

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

Set $\mathbf{a}_h^{k,i} := (\mathbf{d}_h^{k,i+\nu} + \mathbf{l}_h^{k,i+\nu}) - (\mathbf{d}_h^{k,i} + \mathbf{l}_h^{k,i})$ for (adaptively chosen) $\nu > 0$ additional algebraic solvers steps; $R^{k,i+\nu} \rightsquigarrow \rho_h^{k,i}$.

Flux reconstructions

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Verification of the assumptions

Lemma (Assumptions A and B)

Assumptions A and B hold.

Comments

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

Lemma (Assumption C)

Assumption C holds.

Comments

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

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Summary

Discretization methods

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

Linearizations

- fixed point
- Newton

Linear solvers

- independent of the linear solver

... all Assumptions A to C verified

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Outline

Numerical experiment I

Model problem

- p-Laplacian

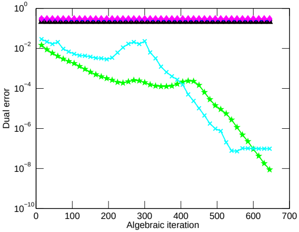
$$\begin{aligned} \nabla\cdot(|\nabla u|^{p-2}\nabla u) &= f && \text{in } \Omega, \\ u &= u_{\mathrm{D}} && \text{on } \partial\Omega \end{aligned}$$

- weak solution (used to impose the Dirichlet BC)

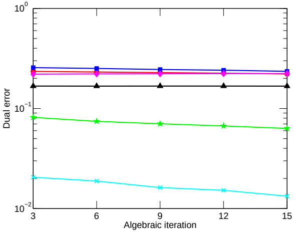
$$u(x,y) = -\frac{p-1}{p}\left((x-\tfrac{1}{2})^2 + (y-\tfrac{1}{2})^2\right)^{\frac{p}{2(p-1)}} + \frac{p-1}{p}\left(\frac{1}{2}\right)^{\frac{p}{p-1}}$$

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

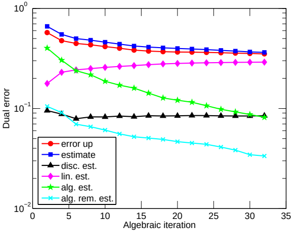
Error and estimators as a function of CG iterations, $p = 10$, 6th level mesh, 6th Newton step.



Newton

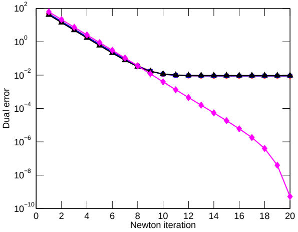


inexact Newton

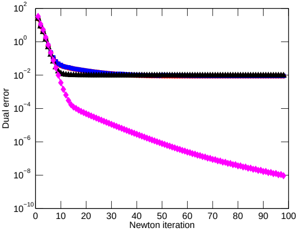


ad. inexact Newton

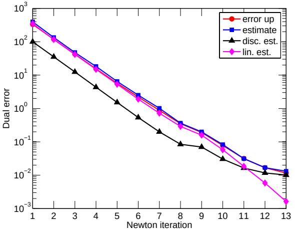
Error and estimators as a function of Newton iterations, $p = 10$, 6th level mesh



Newton

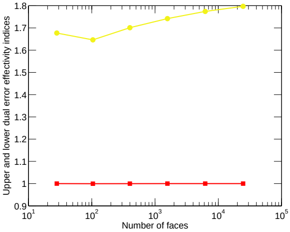


inexact Newton

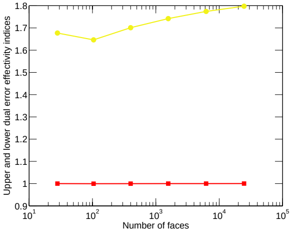


ad. inexact Newton

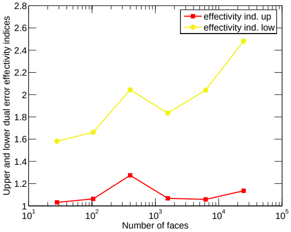
Effectivity indices, $p = 10$



Newton

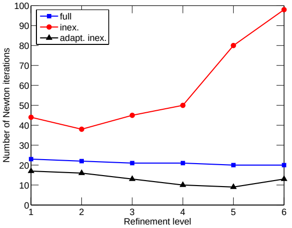


inexact Newton

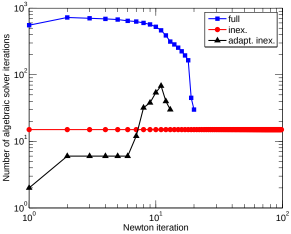


ad. inexact Newton

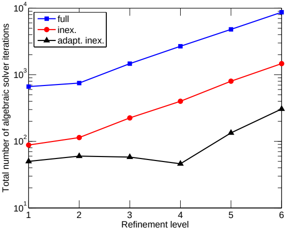
Newton and algebraic iterations, $p = 10$



Newton it. / refinement



alg. it. / Newton step



alg. it. / refinement

Numerical experiment II

Model problem

- p-Laplacian

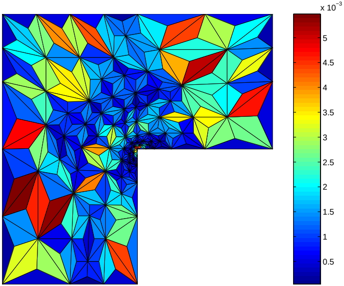
$$\nabla\cdot(|\nabla u|^{p-2}\nabla u) = f \qquad \text{in } \Omega,$$
$$u = u_{\mathrm{D}} \qquad \text{on } \partial\Omega$$

- weak solution (used to impose the Dirichlet BC)

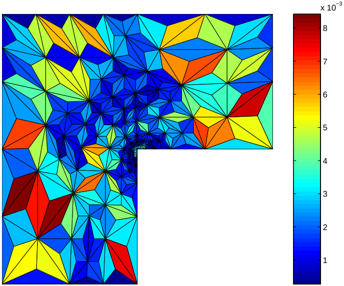
$$u(r,\theta) = r^{\frac{7}{8}} \sin(\theta \tfrac{7}{8})$$

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

Error distribution on an adaptively refined mesh

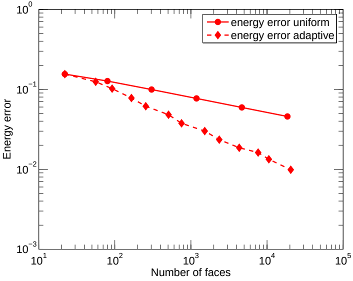


Estimated error distribution

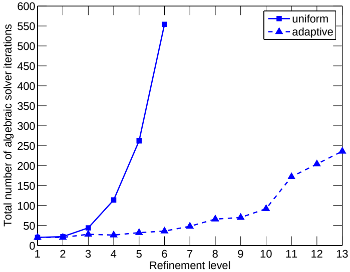


Exact error distribution

Energy error and overall performance



Energy error



Overall performance

Outline

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
- $u_0 \in L^2(\Omega)$, $f \in L^2(0,T;L^2(\Omega))$

Context

- Ph.D. thesis of Soleiman Yousef
- collaboration with IFP Energies Nouvelles

The Stefan problem

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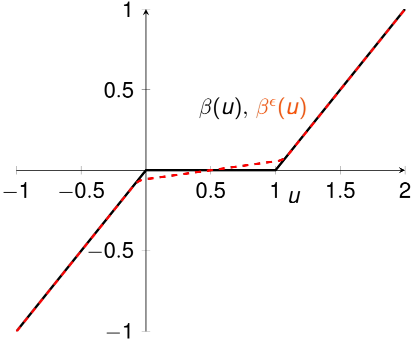
Numerical practice: regularization

Regularization of β, parameter ϵ



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 $\|u|_{I_n} - u_h^{n,\epsilon,k,i}\|$ on time step n, space mesh $\mathcal{K}^n$, regularization parameter ϵ, linearization 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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Setting

Functional spaces

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

Weak formulation

$u \in Z$ with $\beta(u) \in X$,

$u(\cdot, 0) = u_0$ in Ω,

$\langle \partial_t u, \varphi \rangle(s) + (\nabla \beta(u), \nabla \varphi)(s) = (f, \varphi)(s) \quad \forall \varphi \in H^1_0(\Omega), s \in (0, T)$

Approximate solution (with linearization and regularization)

$$u^{\epsilon,k}_{h\tau} \in Z, \qquad \partial_t u^{\epsilon,k}_{h\tau} \in L^2(0, T; L^2(\Omega)), \qquad \beta(u^{\epsilon,k}_{h\tau}) \in X,$$

$$u^{\epsilon,k}_{h\tau}|_{I_n} \text{ is affine in time on } I_n \qquad \forall 1 \leq n \leq N$$

Residual $\mathcal{R}(u^{\epsilon,k}_{h\tau}) \in X'$ **and its dual norm,** $\varphi \in X$

$$\langle \mathcal{R}(u^{\epsilon,k}_{h\tau}), \varphi \rangle_{X',X} := \int_0^T \left\{ \langle \partial_t (u - u^{\epsilon,k}_{h\tau}), \varphi \rangle + (\nabla(\beta(u) - \beta(u^{\epsilon,k}_{h\tau})), \nabla \varphi) \right\}(s) \mathrm{d}s,$$

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

Setting

Functional spaces

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

Weak formulation

$$u \in Z \qquad \text{with } \beta(u) \in X,$$
$$u(\cdot,0) = u_0 \qquad \text{in } \Omega,$$
$$\langle \partial_t u, \varphi\rangle(s) + (\nabla\beta(u), \nabla\varphi)(s) = (f,\varphi)(s) \quad \forall \varphi \in H_0^1(\Omega), s \in (0,T)$$

Approximate solution (with linearization and regularization)

$$u_{h\tau}^{\epsilon,k} \in Z, \qquad \partial_t u_{h\tau}^{\epsilon,k} \in L^2(0,T;L^2(\Omega)), \qquad \beta(u_{h\tau}^{\epsilon,k}) \in X,$$
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$$\langle \partial_t u, \varphi \rangle(s) + (\nabla \beta(u), \nabla \varphi)(s) = (f,\varphi)(s) \quad \forall \varphi \in H_0^1(\Omega), s \in (0,T)$$

Approximate solution (with linearization and regularization)

$$u_{h\tau}^{\epsilon,k} \in Z, \qquad \partial_t u_{h\tau}^{\epsilon,k} \in L^2(0,T;L^2(\Omega)), \qquad \beta(u_{h\tau}^{\epsilon,k}) \in X,$$
$$u_{h\tau}^{\epsilon,k}|_{I_n} \text{ is affine in time on } I_n \qquad \forall 1 \le n \le N$$

Residual $\mathcal{R}(u_{h\tau}^{\epsilon,k}) \in X'$ **and its dual norm**, $\varphi \in X$

$$\langle \mathcal{R}(u_{h\tau}^{\epsilon,k}), \varphi \rangle_{X',X} := \int_0^T \Big\{ \langle \partial_t (u - u_{h\tau}^{\epsilon,k}), \varphi \rangle + (\nabla(\beta(u) - \beta(u_{h\tau}^{\epsilon,k})), \nabla \varphi) \Big\}(s) \mathrm{d}s,$$

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

Setting

Functional spaces

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

Weak formulation

$$u \in Z \qquad \text{with } \beta(u) \in X,$$
$$u(\cdot,0) = u_0 \qquad \text{in } \Omega,$$
$$\langle \partial_t u, \varphi\rangle(s) + (\nabla\beta(u), \nabla\varphi)(s) = (f,\varphi)(s) \quad \forall \varphi \in H_0^1(\Omega), s \in (0,T)$$

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Outline

Estimate distinguishing different error components

Assumption A (Equilibrated flux reconstruction)

For all $n \geq 1$, $k \geq 1$, and $\epsilon > 0$, there exists $\mathbf{t}_h^{n,\epsilon,k} \in \mathbf{H}(\mathrm{div};\Omega)$ s.t.

$$(\nabla\cdot\mathbf{t}_h^{n,\epsilon,k}, 1)_K = (f^n, 1)_K - (\partial_t u_h^{n,\epsilon,k}, 1)_K \qquad \forall K \in \mathcal{K}^n.$$

Theorem (An estimate distinguishing the error components)

Let Assumption A hold. Then, for any $n \geq 1$, $k \geq 1$, and $\epsilon > 0$,

$$\|\mathcal{R}(u_h^{n,\epsilon,k})\|_{X_n'} \leq \eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k} + \eta_{\mathrm{lin}}^{n,\epsilon,k}.$$

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

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

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

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

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

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Estimate distinguishing different error components

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

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

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

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Efficiency assumptions

Assumption B (Technicalities)

All the meshes are shape-regular and all the approximations are piecewise polynomial.

Residual estimators

$$\left(\eta_{\mathrm{res},1}^{n,\epsilon_n,k_n}\right)^2 := \tau^n \sum_{K\in\mathcal{K}^{n-1,n}} h_K^2 \|f^n - \partial_t u_h^{n,\epsilon_n,k_n} + \nabla\cdot \mathbf{l}_h^{n,\epsilon_n,k_n}\|_K^2,$$

$$\left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2 := \tau^n \sum_{F\in\mathcal{F}^{\mathrm{i},n-1,n}} h_F \|[\![\mathbf{l}_h^{n,\epsilon_n,k_n}]\!]\cdot\mathbf{n}_F\|_F^2$$

Assumption C (Approximation property)

For all $1 \le n \le N$, there holds

$$\tau^n \sum_{K\in\mathcal{K}^{n-1,n}} \|\mathbf{l}_h^{n,\epsilon_n,k_n} + \mathbf{t}_h^{n,\epsilon_n,k_n}\|_K^2 \le C\left(\left(\eta_{\mathrm{res},1}^{n,\epsilon_n,k_n}\right)^2 + \left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2\right).$$

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$$\left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2 := \tau^n \sum_{F\in\mathcal{F}^{\mathrm{i},n-1,n}} h_F \|[\![\mathbf{l}_h^{n,\epsilon_n,k_n}]\!]\cdot\mathbf{n}_F\|_F^2$$

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For all $1 \le n \le N$, *there holds*

$$\tau^n \sum_{K\in\mathcal{K}^{n-1,n}} \|\mathbf{l}_h^{n,\epsilon_n,k_n} + \mathbf{t}_h^{n,\epsilon_n,k_n}\|_K^2 \le C\left(\left(\eta_{\mathrm{res},1}^{n,\epsilon_n,k_n}\right)^2 + \left(\eta_{\mathrm{res},2}^{n,\epsilon_n,k_n}\right)^2\right).$$

Efficiency assumptions

Theorem (Efficiency)

Let, for all $1 \leq n \leq N$, the stopping and balancing criteria be satisfied with the parameters small enough. Let Assumptions B and C hold. Then

$$\eta_{\mathrm{sp}}^{n,\epsilon_n,k_n} + \eta_{\mathrm{tm}}^{n,\epsilon_n,k_n} + \eta_{\mathrm{reg}}^{n,\epsilon_n,k_n} + \eta_{\mathrm{lin}}^{n,\epsilon_n,k_n} \lesssim \|\mathcal{R}(u_h^{n,\epsilon_n,k_n})\|_{X_n'}.$$

Outline

Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

$$\frac{L_\beta}{2}\|u-u_{h\tau}\|^2_{X'}+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)}+\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_T}$$
$$\leq\frac{L_\beta}{2}(2e^T-1)\left(\|\mathcal{R}(u_{h\tau})\|^2_{X'}+\|(u-u_{h\tau})(\cdot,0)\|^2_{H^{-1}(\Omega)}\right)$$

Theorem (Temperature and enthalpy errors, tight Gronwall)

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

$$\frac{L_\beta}{2}\|u-u_{h\tau}\|^2_{X'}+\frac{L_\beta}{2}\|(u-u_{h\tau})(\cdot,T)\|^2_{H^{-1}(\Omega)}+\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_T}$$
$$+2\int_0^T\left(\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_t}+\int_0^t\|\beta(u)-\beta(u_{h\tau})\|^2_{Q_s}e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t$$
$$\leq\frac{L_\beta}{2}\Bigg\{(2e^T-1)\|(u-u_{h\tau})(\cdot,0)\|^2_{H^{-1}(\Omega)}+\|\mathcal{R}(u_{h\tau})\|^2_{X'}$$
$$+2\int_0^T\left(\|\mathcal{R}(u_{h\tau})\|^2_{X'_t}+\int_0^t\|\mathcal{R}(u_{h\tau})\|^2_{X'_s}e^{t-s}\,\mathrm{d}s\right)\mathrm{d}t\Bigg\}.$$

Relation residual–energy norm

Energy estimate (by the Gronwall lemma)

$$\frac{L_\beta}{2}\|u - u_{h\tau}\|^2_{X'} + \frac{L_\beta}{2}\|(u - u_{h\tau})(\cdot, T)\|^2_{H^{-1}(\Omega)} + \|\beta(u) - \beta(u_{h\tau})\|^2_{Q_T}$$
$$\leq \frac{L_\beta}{2}(2e^T - 1)\left(\|\mathcal{R}(u_{h\tau})\|^2_{X'} + \|(u - u_{h\tau})(\cdot, 0)\|^2_{H^{-1}(\Omega)}\right)$$

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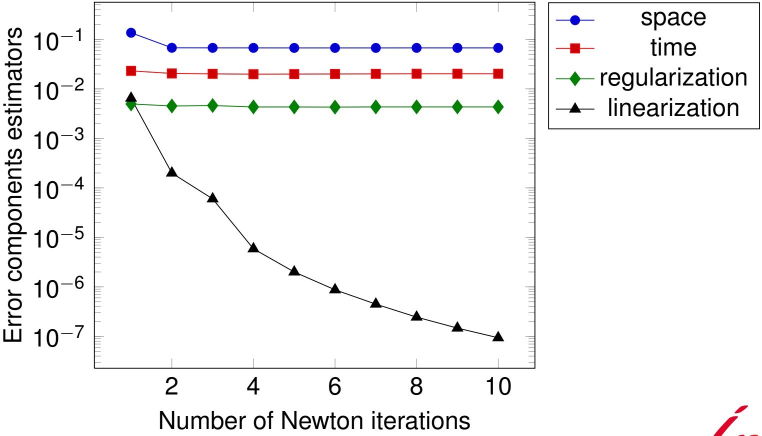
$$+ 2\int_0^T \left(\|\beta(u) - \beta(u_{h\tau})\|^2_{Q_t} + \int_0^t \|\beta(u) - \beta(u_{h\tau})\|^2_{Q_s} e^{t-s}\, \mathrm{d}s\right) \mathrm{d}t$$
$$\leq \frac{L_\beta}{2}\Bigg\{(2e^T - 1)\|(u - u_{h\tau})(\cdot, 0)\|^2_{H^{-1}(\Omega)} + \|\mathcal{R}(u_{h\tau})\|^2_{X'}$$
$$+ 2\int_0^T \left(\|\mathcal{R}(u_{h\tau})\|^2_{X'_t} + \int_0^t \|\mathcal{R}(u_{h\tau})\|^2_{X'_s} e^{t-s}\, \mathrm{d}s\right) \mathrm{d}t\Bigg\}.$$

Outline

Linearization stopping criterion

Linearization stopping criterion

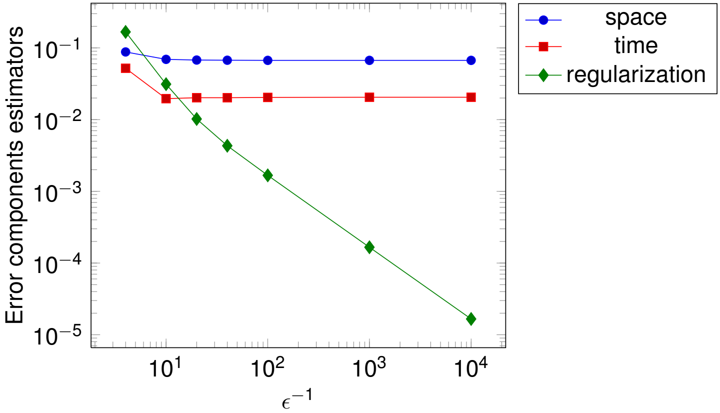
$$\eta_{\mathrm{lin}}^{n,\epsilon,k} \leq \Gamma_{\mathrm{lin}} \left(\eta_{\mathrm{sp}}^{n,\epsilon,k} + \eta_{\mathrm{tm}}^{n,\epsilon,k} + \eta_{\mathrm{reg}}^{n,\epsilon,k} \right)$$



Regularization stopping criterion

Regularization stopping criterion

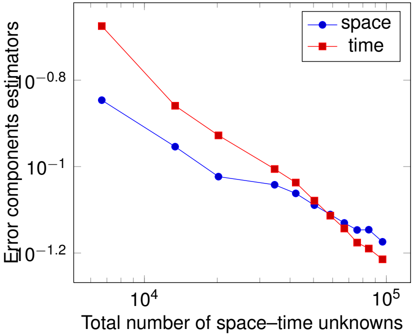
$$\eta_{\mathrm{reg}}^{n,\epsilon,k_n} \leq \Gamma_{\mathrm{reg}} \left(\eta_{\mathrm{sp}}^{n,\epsilon,k_n} + \eta_{\mathrm{tm}}^{n,\epsilon,k_n} \right)$$

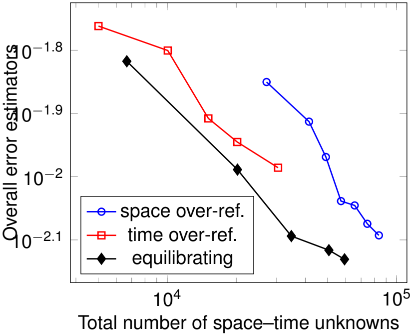


Equilibrating time and space errors

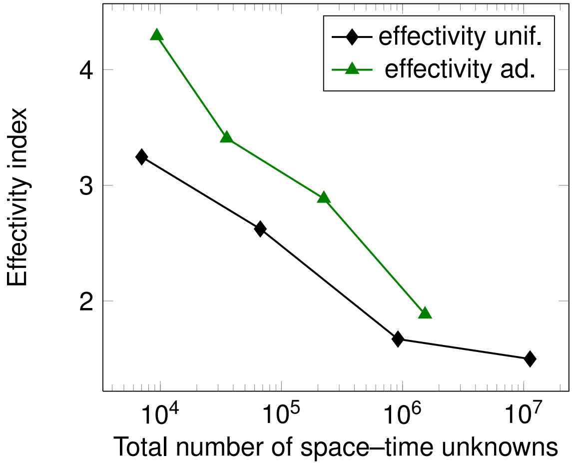
Equilibrating time and space errors

$$\gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon_n,k_n} \le \eta_{\mathrm{tm}}^{n,\epsilon_n,k_n} \le \Gamma_{\mathrm{tm}}\eta_{\mathrm{sp}}^{n,\epsilon_n,k_n}$$

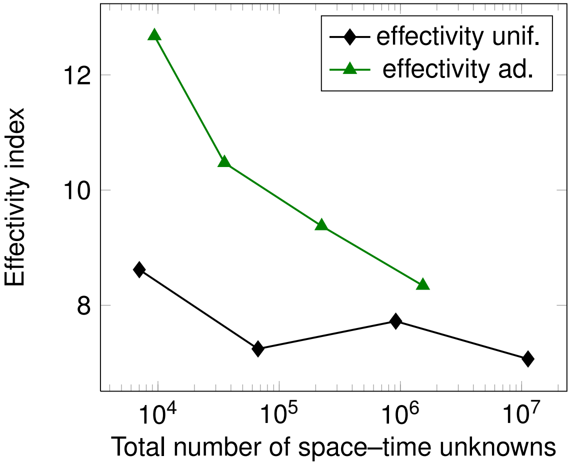




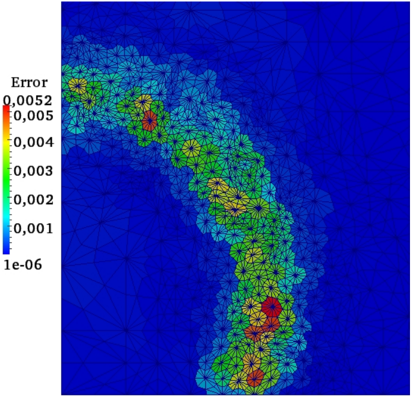
Effectivity indices (dual norm of the residual)

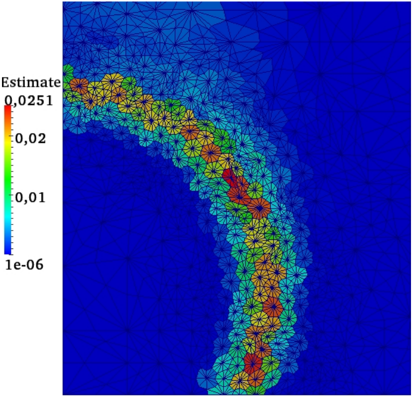


Effectivity indices (energy norm)



Actual and estimated error distribution





Computational efficiency

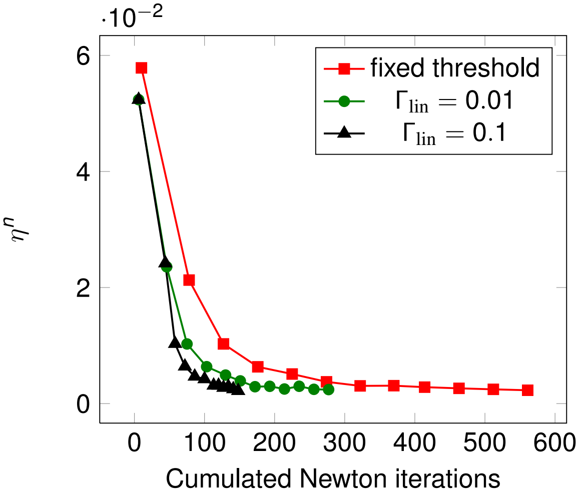


Figure: Number of cumulated Newton iterations vs. error estimate

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Conclusions and future directions

Entire adaptivity

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

Future directions

- other coupled nonlinear systems
- convergence and optimality

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Thank you for your attention!