Adaptivity of error components for optimality in numerical simulations

Martin Vohralík

in collaboration with Ibtihel Ben Gharbia, Jakub Wiktor Both, Jad Dabaghi, Alexandre Ern, François Févotte, Eric Flauraud, Alexander Haberl, Ibtissem Lannabi, Vincent Martin, Koondanibha Mitra, Jan Martin Nordbotten, Jan Papež, Dirk Praetorius, Ari Rappaport, Ulrich Rüde, Tor Harald Sandve, Stefan Schimanko, Peter von Schultzendorff, Mary F. Wheeler, Barbara Wohlmuth, Soleiman Yousef

Inria Paris & Charles University Prague

Prague, October 22, 2026





Outline

1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

Outline

1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

Outline

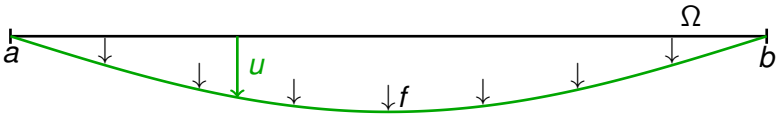
1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

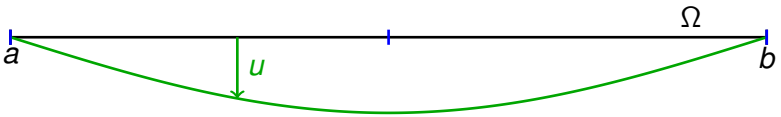
- unknown exact solution u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

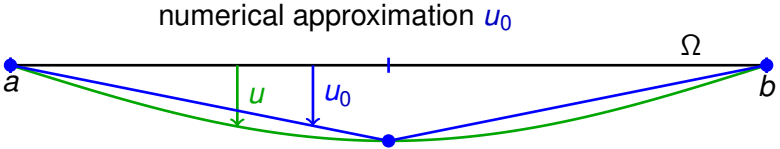
- unknown exact solution u
- computational mesh $\mathcal{T}_0$



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

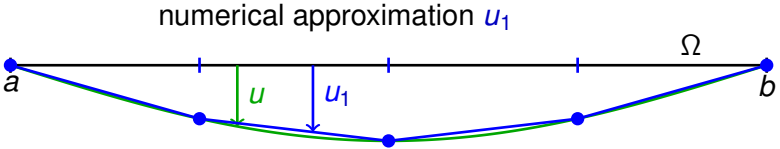
- unknown exact solution u
- computational mesh $\mathcal{T}_0$



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

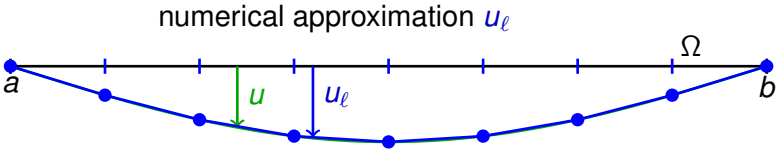
- unknown exact solution u
- computational mesh $\mathcal{T}_1$



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$

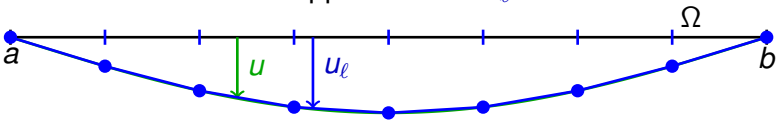


PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources**

  $\Rightarrow$ numerical approximation u_ℓ **closer** to u

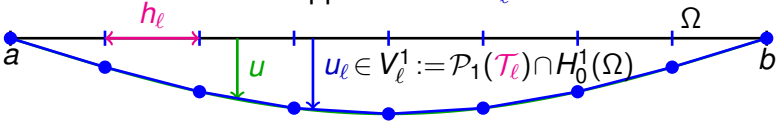


PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources**

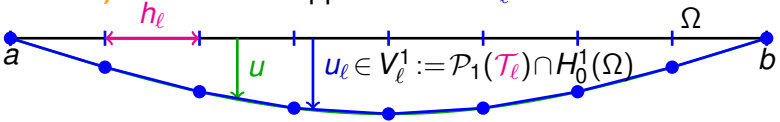
$\Rightarrow$ numerical approximation u_ℓ **closer** to u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

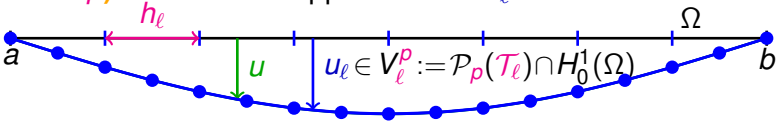
- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$)**
) $\Rightarrow$ numerical approximation u_ℓ closer to u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

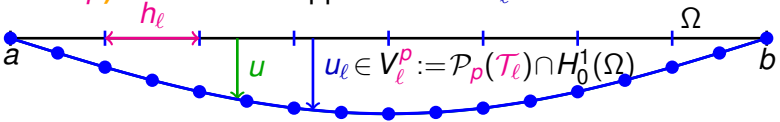
- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



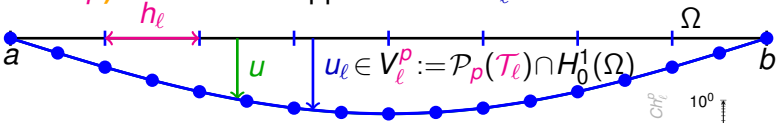
Textbook numerical analysis

- $\|(u - u_\ell)'\| \leq C h_\ell^p$ when $u \in H^{p+1}(\Omega)$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

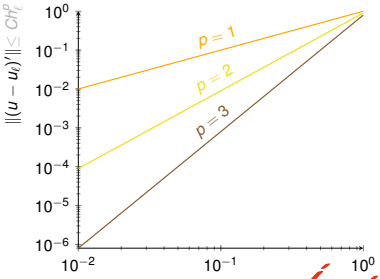
Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Textbook numerical analysis

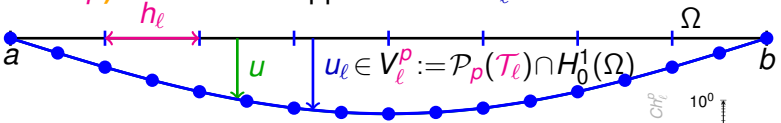
- $\|(u - u_\ell)'\| \leq C h_\ell^p$ when $u \in H^{p+1}(\Omega)$



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

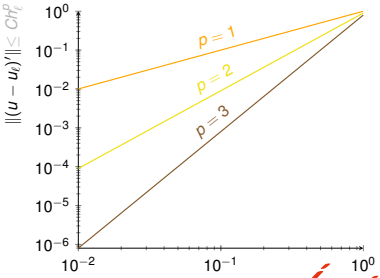
Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Textbook numerical analysis

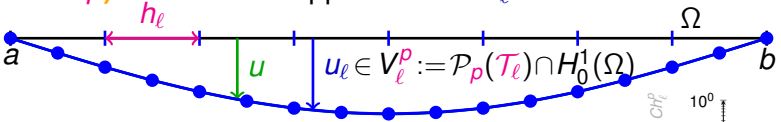
- $\|(u - u_\ell)'\| \leq C h_\ell^p$ when $u \in H^{p+1}(\Omega)$
- when $u \in H^s(\Omega)$: only $h_\ell^{(s-1)}$



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

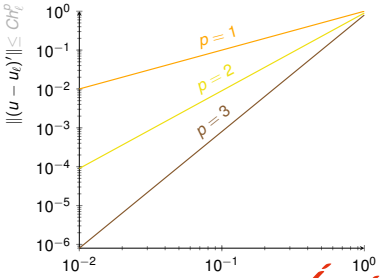
Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Textbook numerical analysis

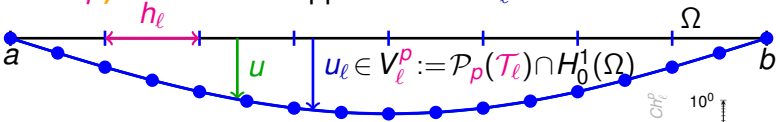
- $\|(u - u_\ell)'\| \leq C h_\ell^p$ when $u \in H^{p+1}(\Omega)$
- when $u \in H^s(\Omega)$: only $h_\ell^{(s-1)}$
  1. **convergence rate limited by regularity**



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

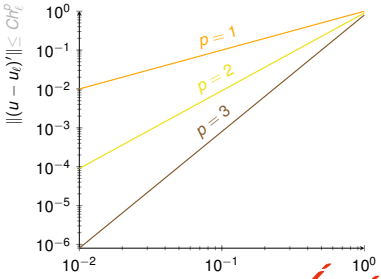
Textbook numerical approximation

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources (refinement of $\mathcal{T}_\ell$ ($h_\ell \searrow 0$) and/or increase of p)** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Textbook numerical analysis

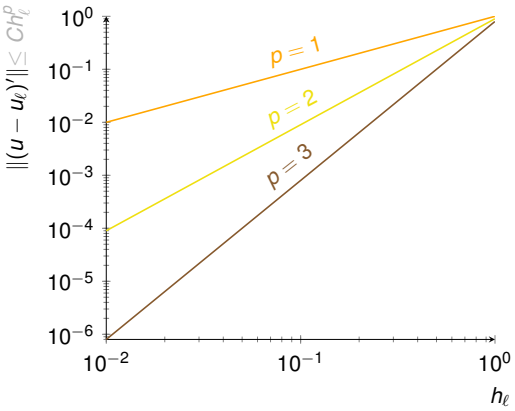
- $\|(u - u_\ell)'\| \leq C h_\ell^p$ when $u \in H^{p+1}(\Omega)$
- when $u \in H^s(\Omega)$: only $h_\ell^{(s-1)}$
  1. **convergence rate limited by regularity**
  2. **convergence rate same for small and big p**



Outline

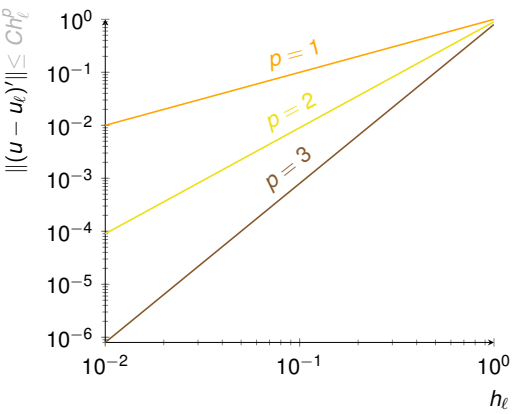
1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

Convergence for **regular** problems

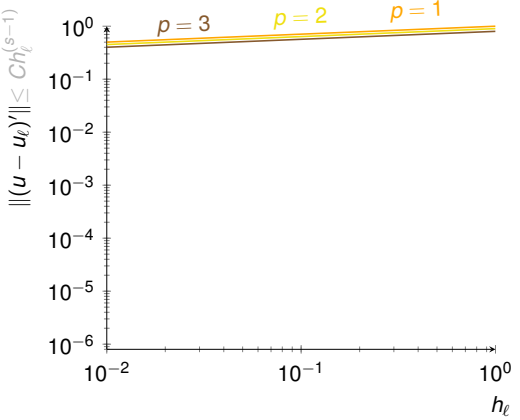


$u \in H^{p+1}(\Omega)$

Convergence for **regular** and **singular** problems

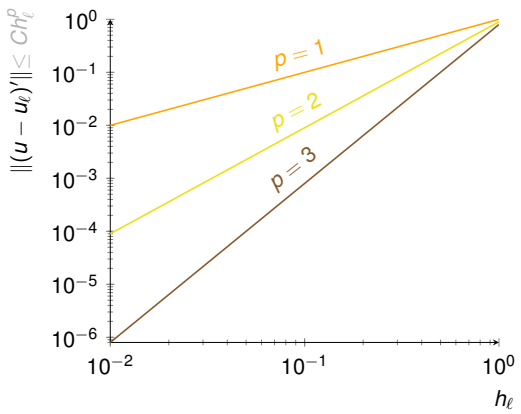


$u \in H^{p+1}(\Omega)$

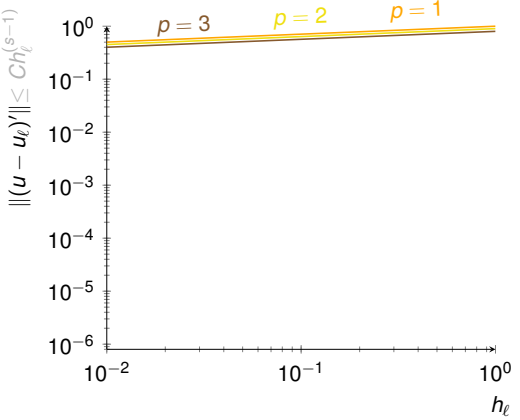


$u \in H^s(\Omega)$, $s = 1.15$

Convergence for **regular** and **singular** problems



$u \in H^{p+1}(\Omega)$

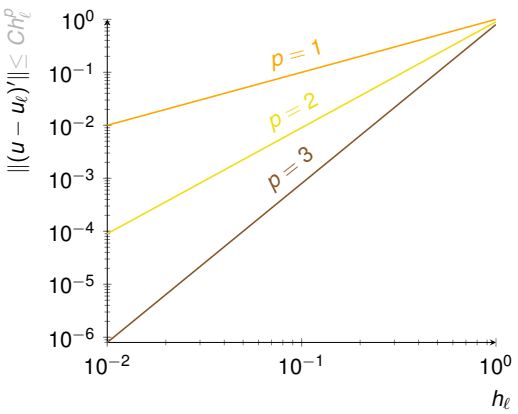


$u \in H^s(\Omega)$, $s = 1.15$

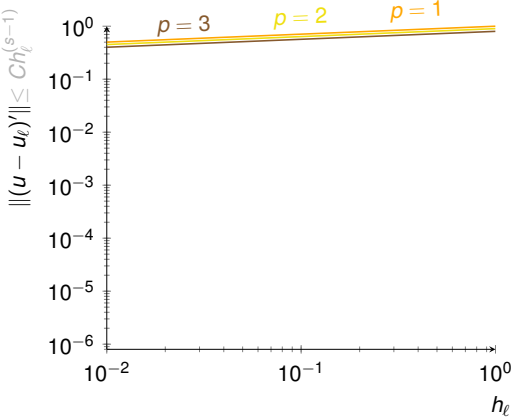
Common claim

High-order finite elements do not pay-off for low-regularity solutions.

Convergence for **regular** and **singular** problems



$u \in H^{p+1}(\Omega)$

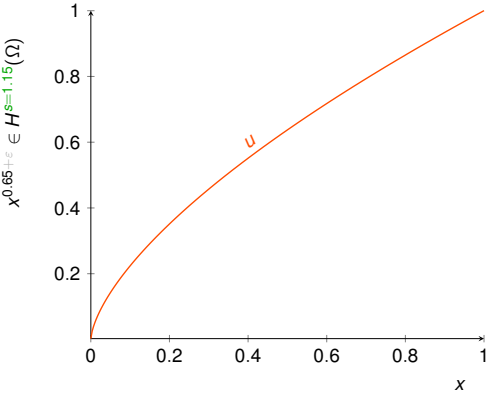


$u \in H^s(\Omega)$, $s = 1.15$

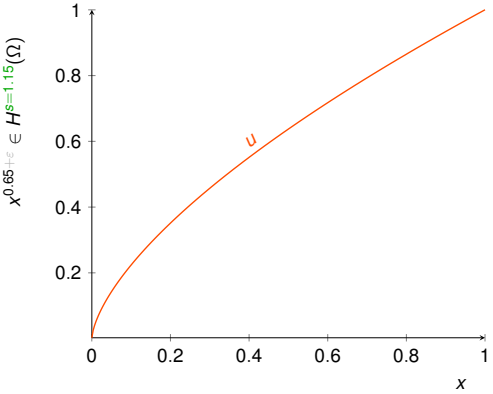
Common claim: uniform mesh refinement

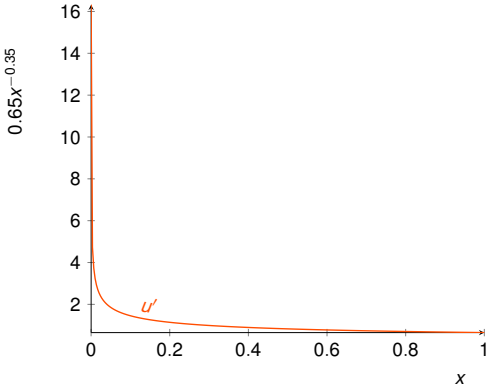
High-order finite elements do not pay-off for low-regularity solutions.

Convergence for **regular** and **singular** problems

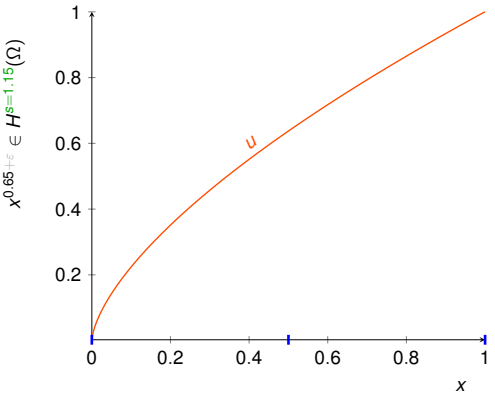


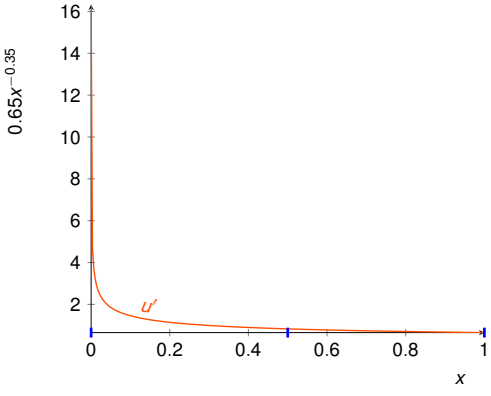
Convergence for **regular** and **singular** problems



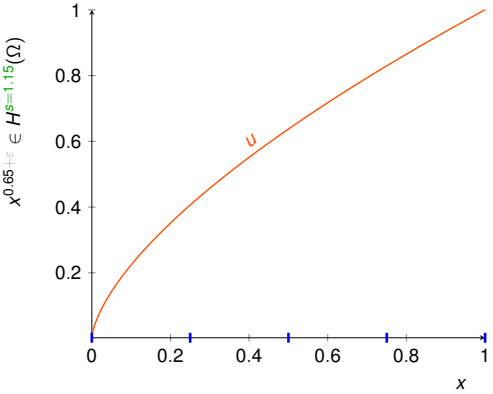


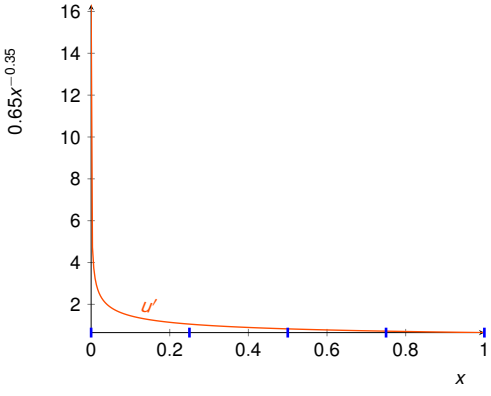
Convergence for **regular** and **singular** problems



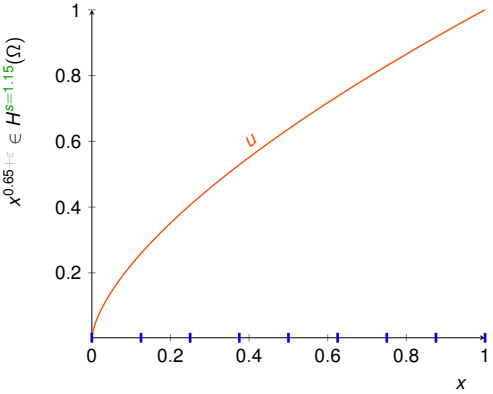


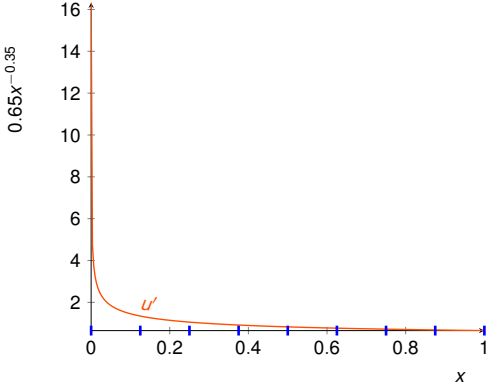
Convergence for **regular** and **singular** problems



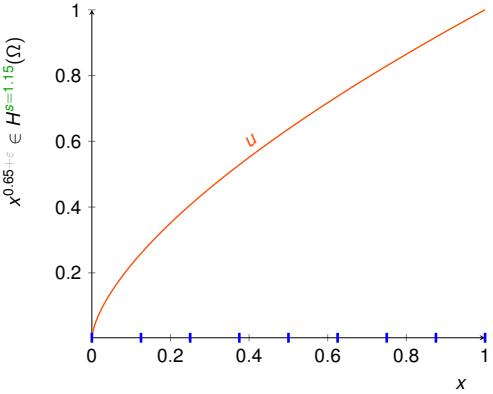


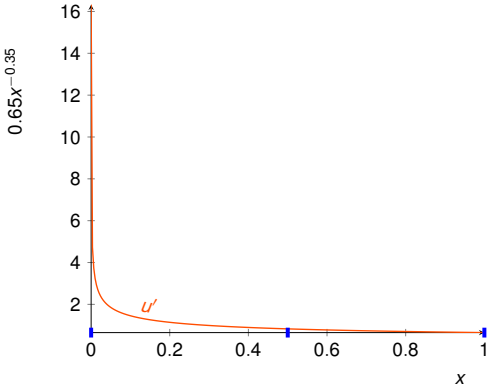
Convergence for **regular** and **singular** problems



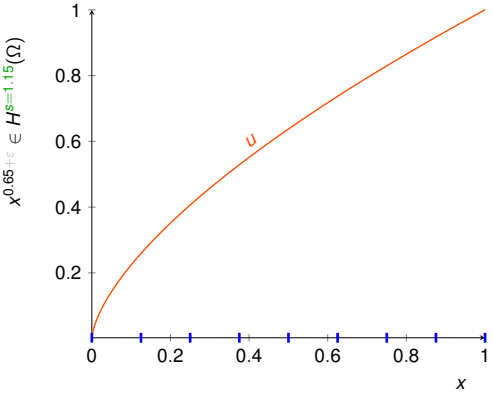


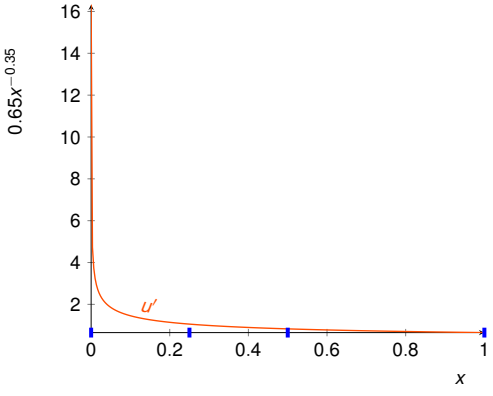
Convergence for **regular** and **singular** problems



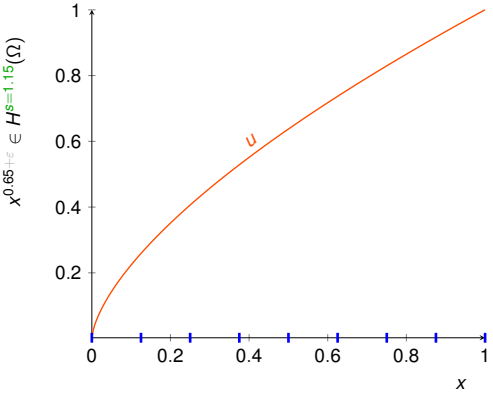


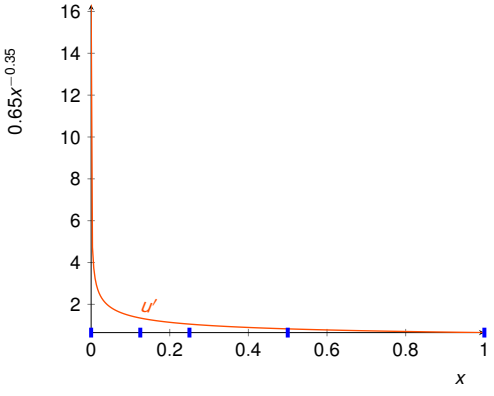
Convergence for **regular** and **singular** problems



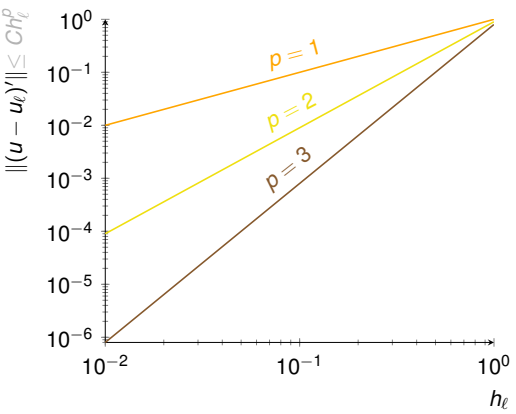


Convergence for **regular** and **singular** problems

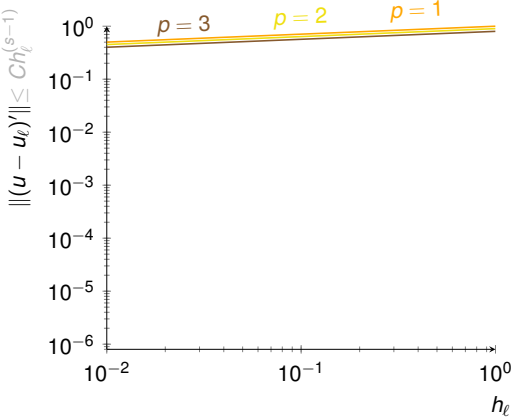




Convergence for **regular** and **singular** problems

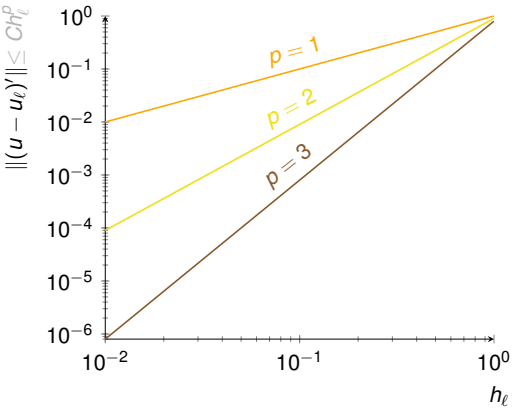


$u \in H^{p+1}(\Omega)$

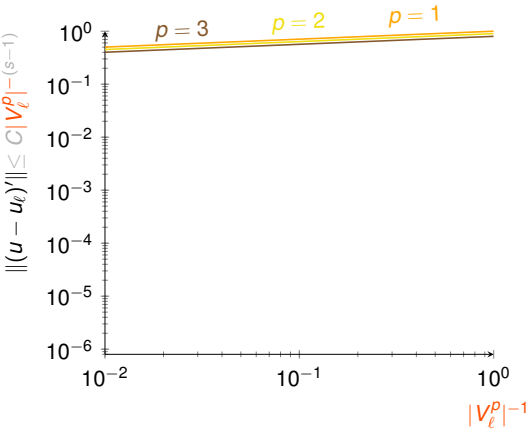


$u \in H^s(\Omega)$, $s = 1.15$

Convergence for **regular** and **singular** problems

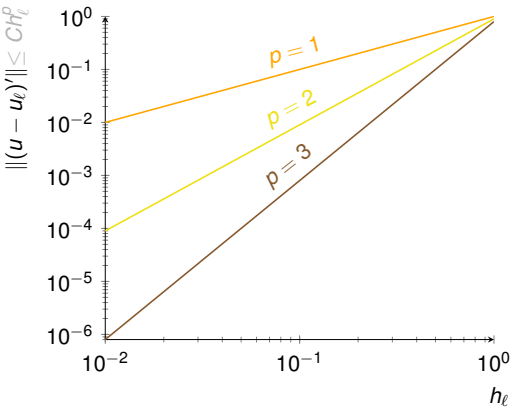


$u \in H^{p+1}(\Omega)$

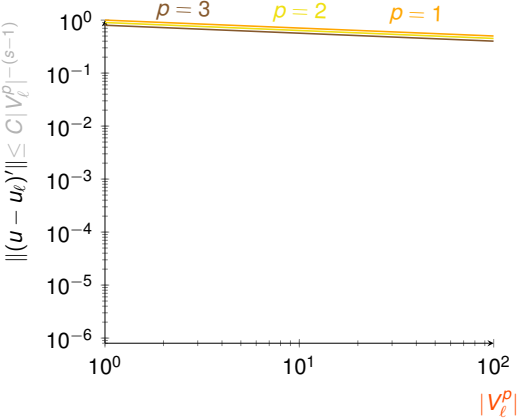


$u \in H^s(\Omega)$, $s = 1.15$, $h_\ell \approx |V_\ell^p|^{-1}$

Convergence for **regular** and **singular** problems

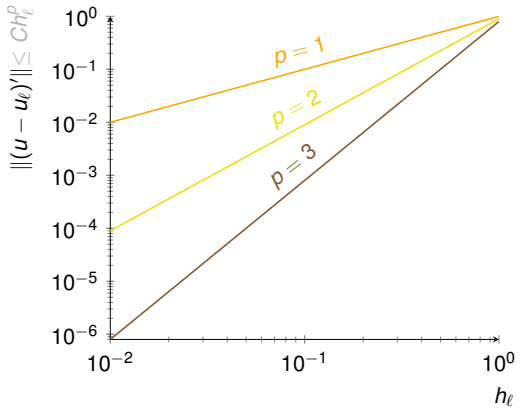


$u \in H^{p+1}(\Omega)$

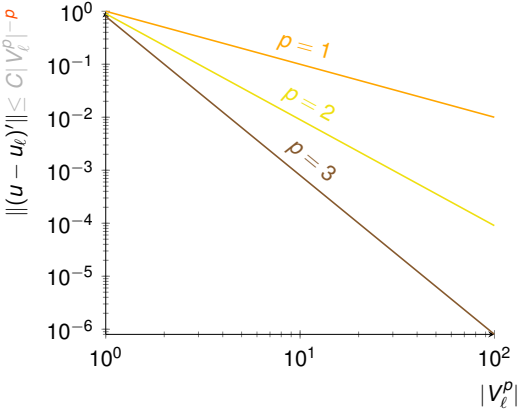


$u \in H^s(\Omega)$, $s = 1.15$

Convergence for **regular** and **singular** problems: **adaptivity**

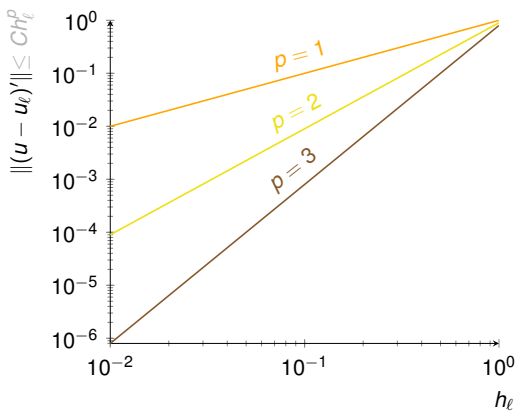


$u \in H^{p+1}(\Omega)$

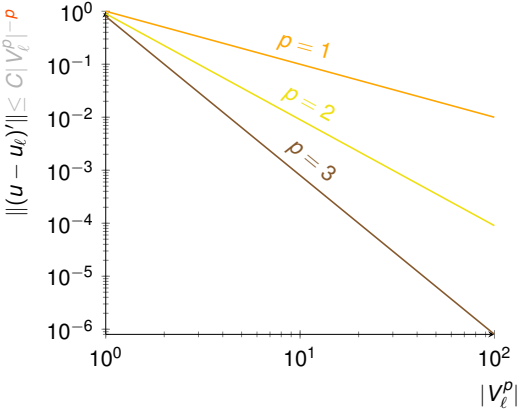


$u \in H^s(\Omega)$, $s = 1.15$

Convergence for **regular** and **singular** problems: **adaptivity**



$u \in H^{p+1}(\Omega)$

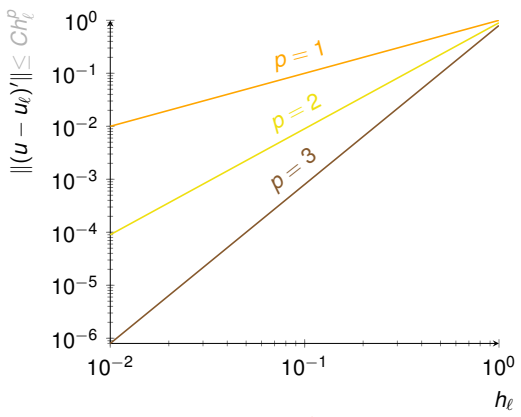


$u \in H^s(\Omega)$, $s = 1.15$

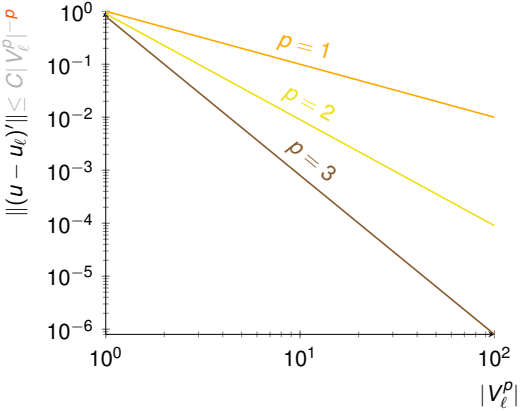
Rectified claim

High-order finite elements always pay-off.

Convergence for **regular** and **singular** problems: **adaptivity**



$u \in H^{p+1}(\Omega)$



$u \in H^s(\Omega)$, $s = 1.15$

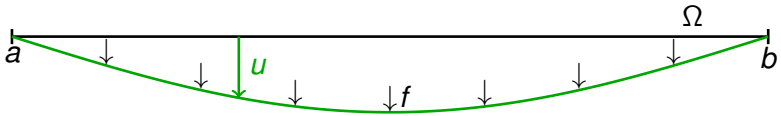
Rectified claim: adaptive mesh refinement

High-order finite elements always pay-off.

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

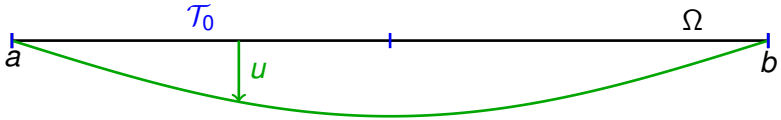
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u



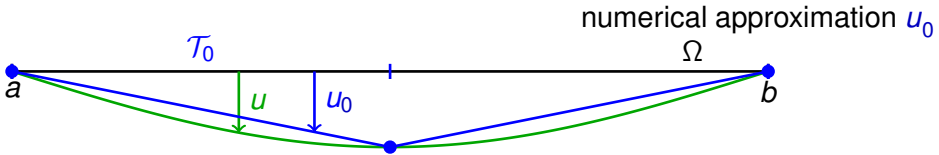
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_0$



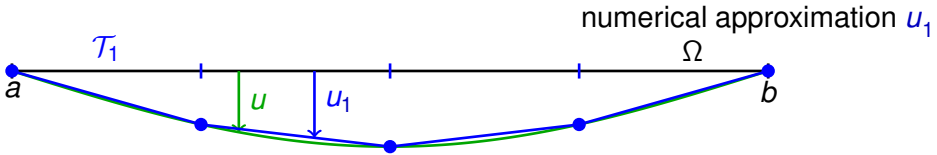
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_0$



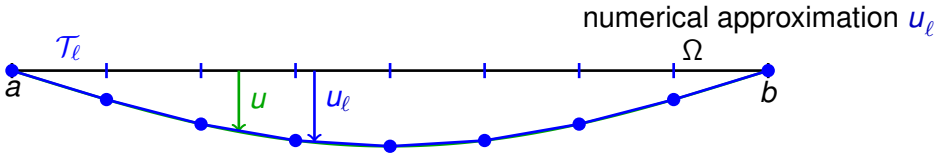
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_1$



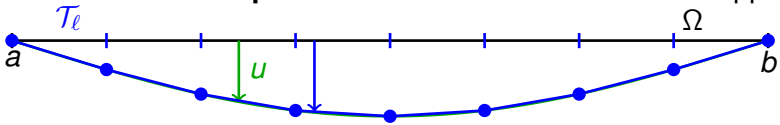
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$



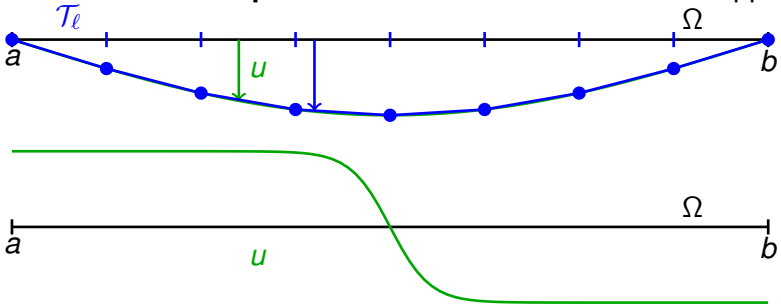
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



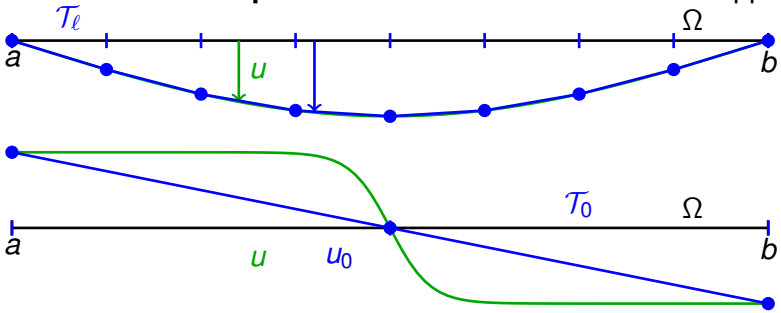
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



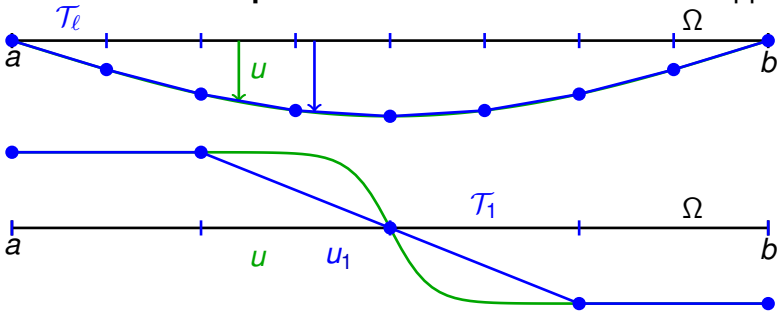
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



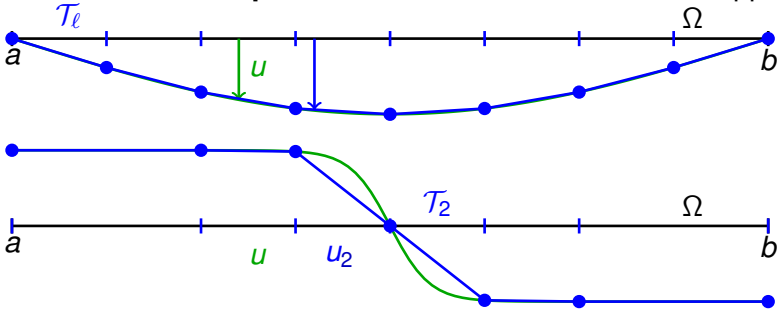
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



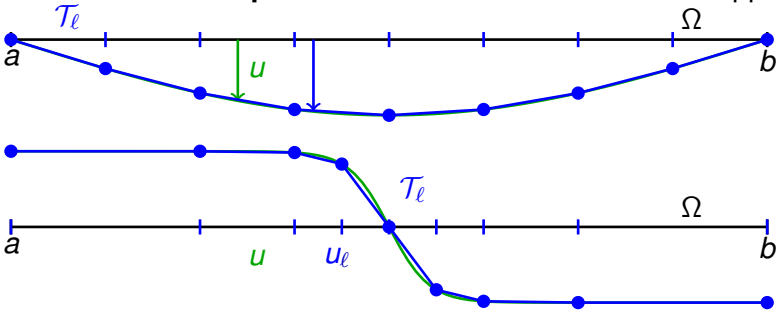
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



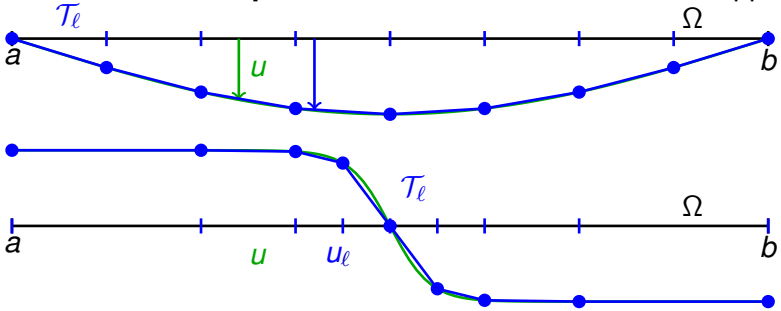
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



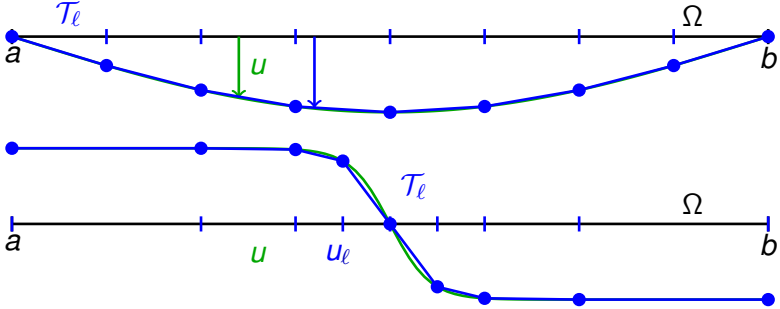
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

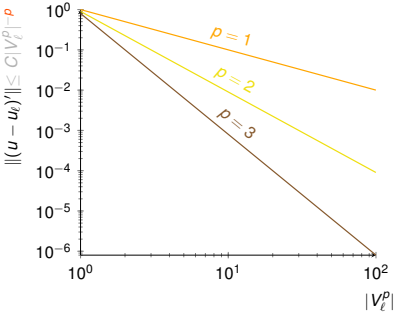
- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

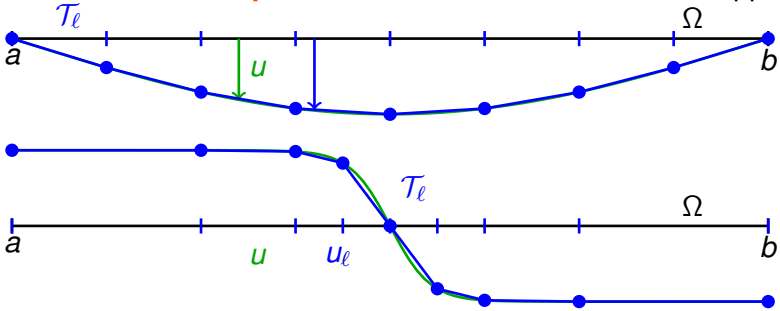
- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u





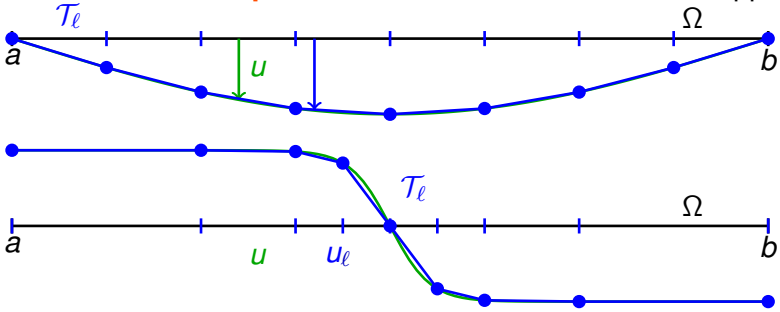
PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u

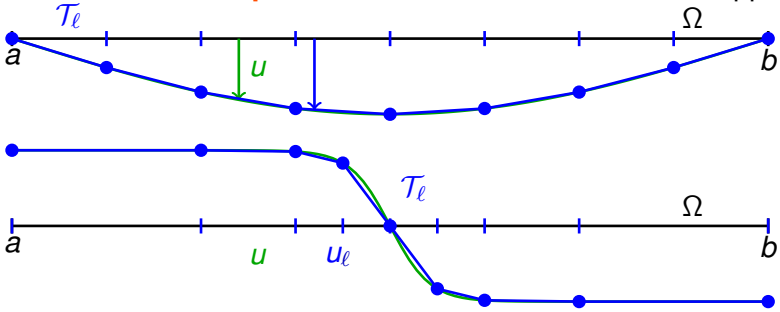


Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Need to solve

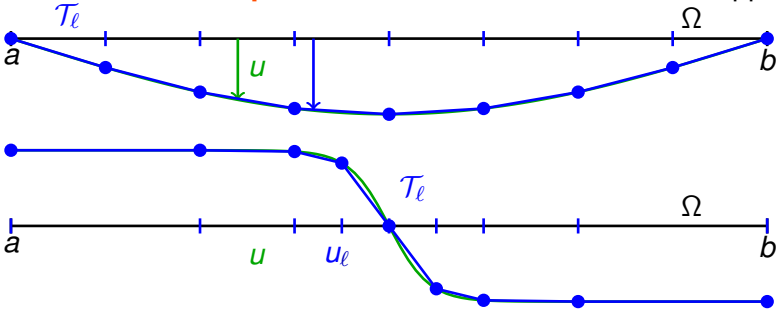
$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

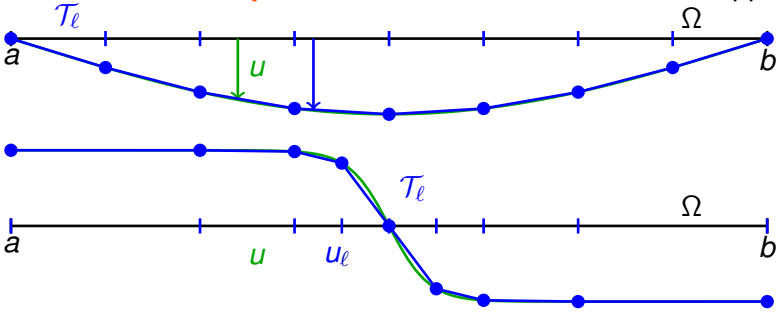
$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

Algebraic error

$\|(u_\ell - u_\ell^i)'\|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ^i **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

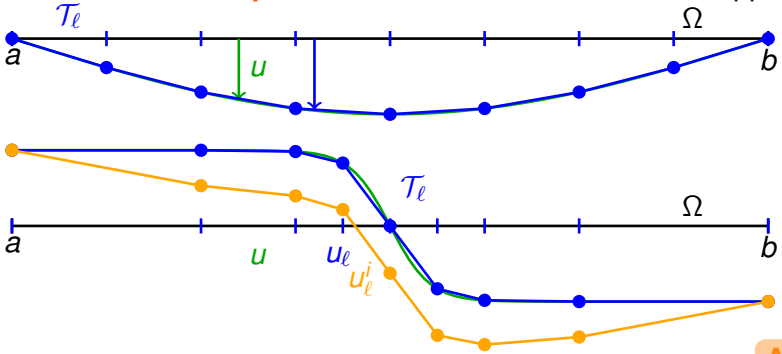
$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{j} |V_\ell^p|$

Algebraic error

$\|(u_\ell - u_\ell^i)'\|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ^i **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

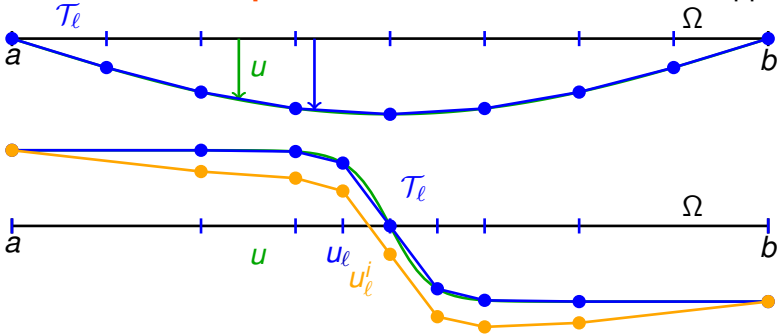
$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

Algebraic error

$\|(u_\ell - u_\ell^i)'\|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ^i **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

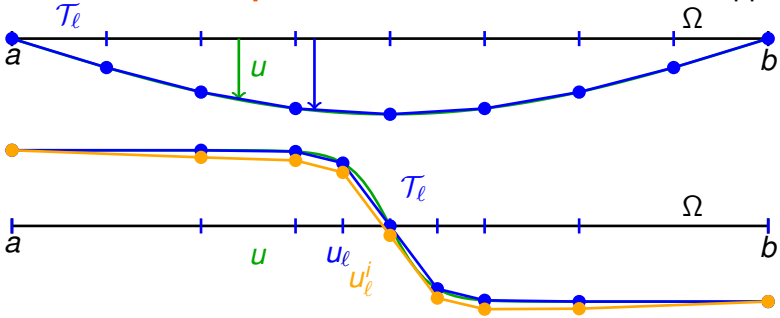
$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

Algebraic error

$\|(u_\ell - u_\ell^i)'\|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ^i **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

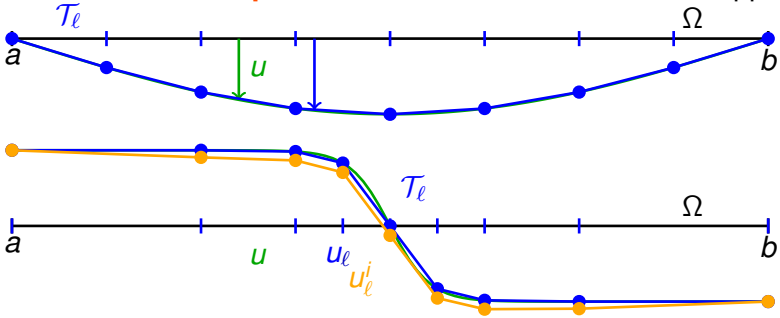
$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

Algebraic error

$\|(u_\ell - u_\ell^i)'\|$

PDE example: find $u : (a, b) \to \mathbb{R}$ s.t. $-u'' = f$ in (a, b), $u = 0$ in a, b

- unknown exact solution u
- computational mesh $\mathcal{T}_\ell$ **(adaptively refined)**
- **more computational resources** $\Rightarrow$ numerical approximation u_ℓ^i **closer** to u



Need to solve

$\mathbb{A}_\ell \mathbf{U}_\ell = \mathbf{F}_\ell$

Cost

$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$

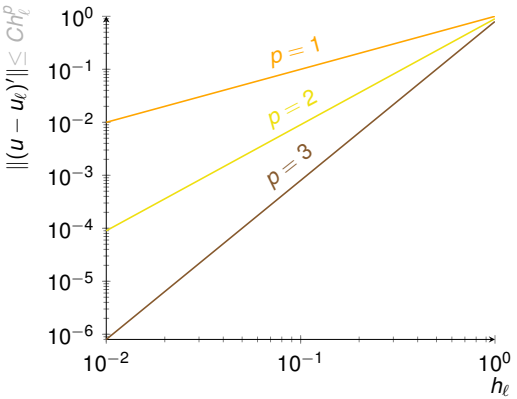
Total error

$\|(u - u_{\bar{\ell}}^{\bar{i}})'\|$

Algebraic error

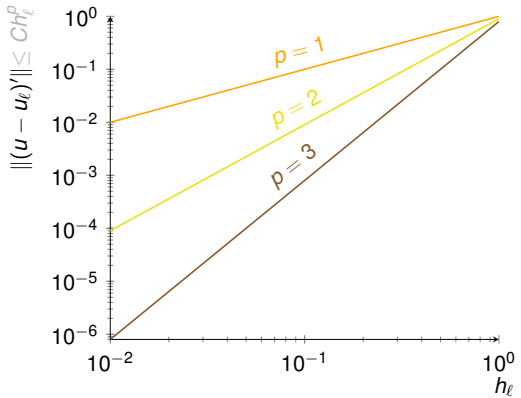
$\|(u_\ell - u_\ell^i)'\|$

Adaptivity of error components: optimality in numerical simulations

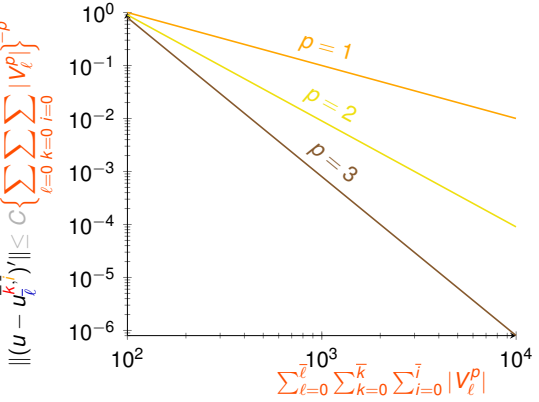


$u \in H^{p+1}(\Omega)$

Adaptivity of error components: optimality in numerical simulations

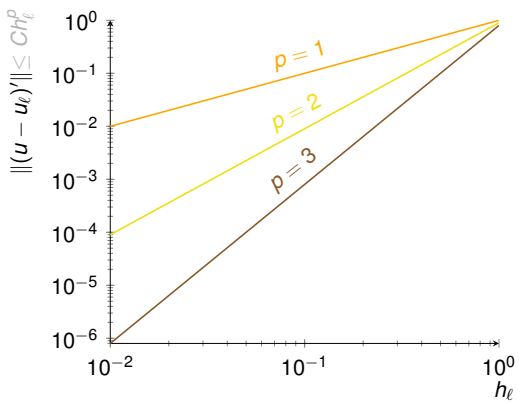


$u \in H^{p+1}(\Omega)$

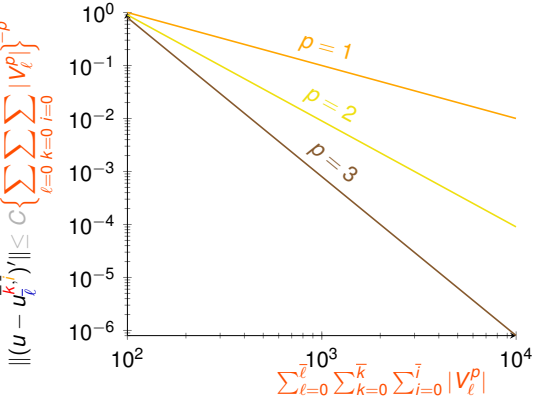


$u \in H^s(\Omega)$, $s = 1.15$

Adaptivity of error components: optimality in numerical simulations



$u \in H^{p+1}(\Omega)$



$u \in H^s(\Omega)$, $s = 1.15$

Optimality with respect to the **cost**

It is impossible to design an algorithm with better convergence rate.

Outline

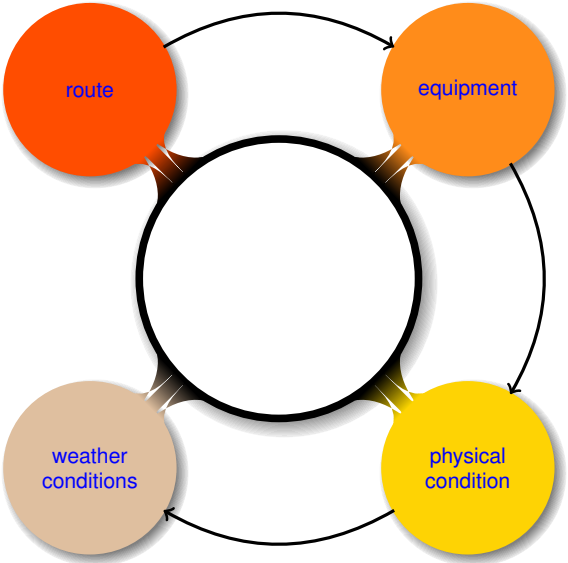
1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

Control the error and act adaptively: real life

Control the error and act adaptively: real life

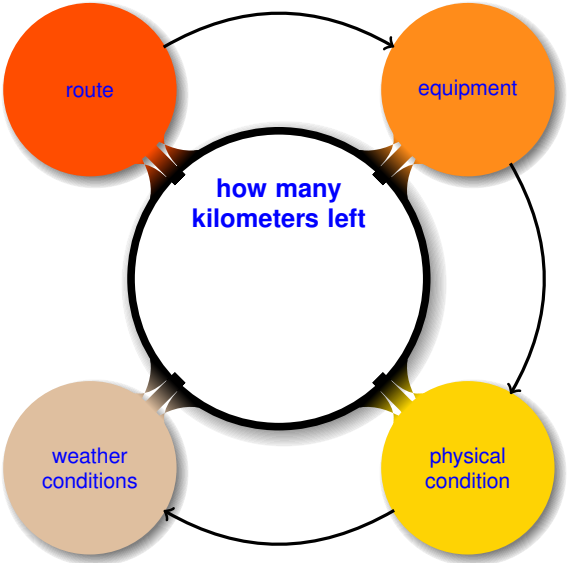
wandering Paris–Santiago de Compostela

Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

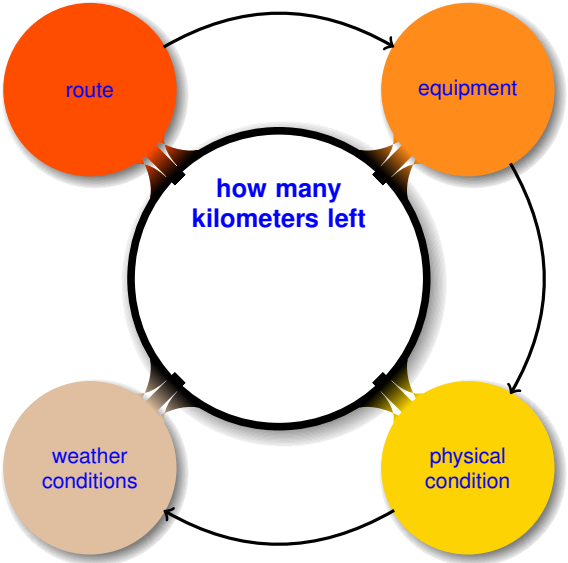
Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

$\Longleftarrow$ control the error

Control the error and act adaptively: real life



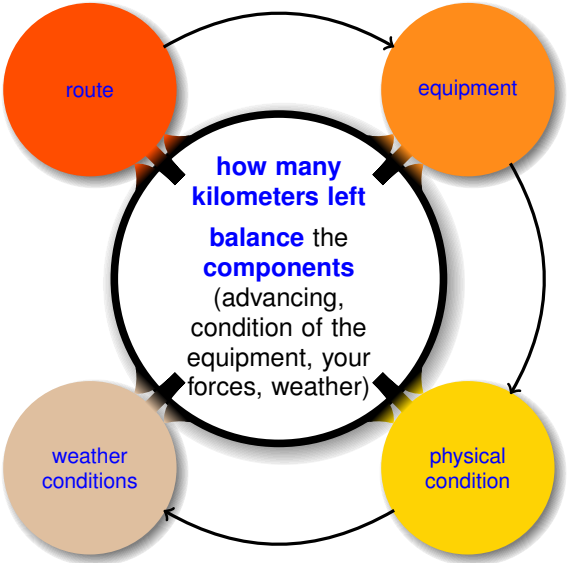
wandering Paris–Santiago de Compostela

$\Leftarrow$ control the error

possible since

- target known
-

Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

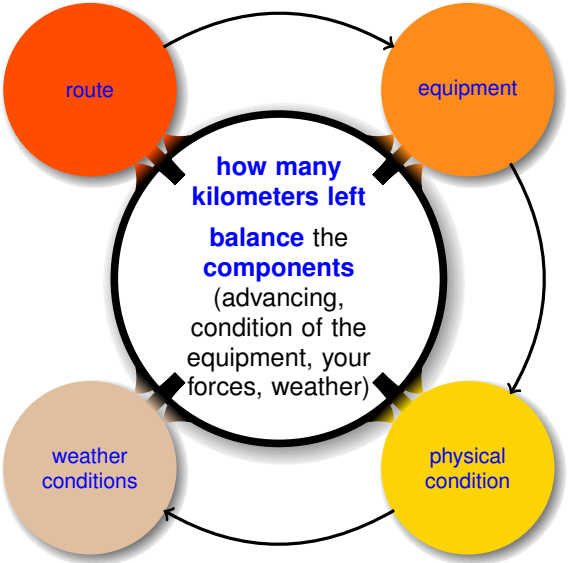
$\Leftarrow$ control the error

$\Leftarrow$ act adaptively

possible since

- target known
-

Control the error and act adaptively: real life



wandering Paris–Santiago de Compostela

$\Leftarrow$ control the error

$\Leftarrow$ act adaptively

possible since

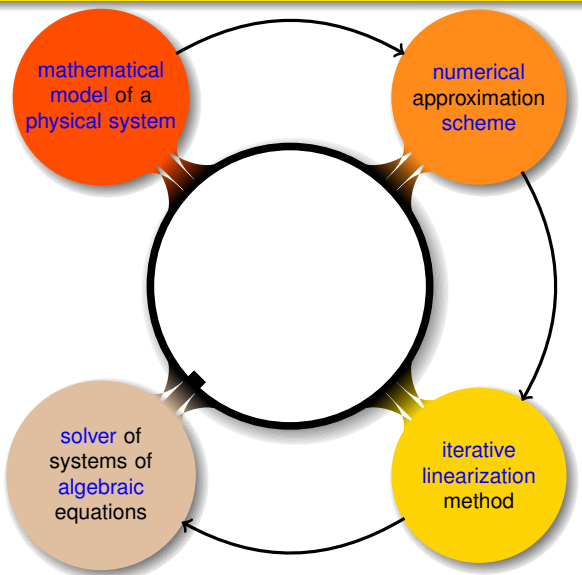
- target known
- components known

Control the error and act adaptively: numerical simulations

Control the error and act adaptively: numerical simulations

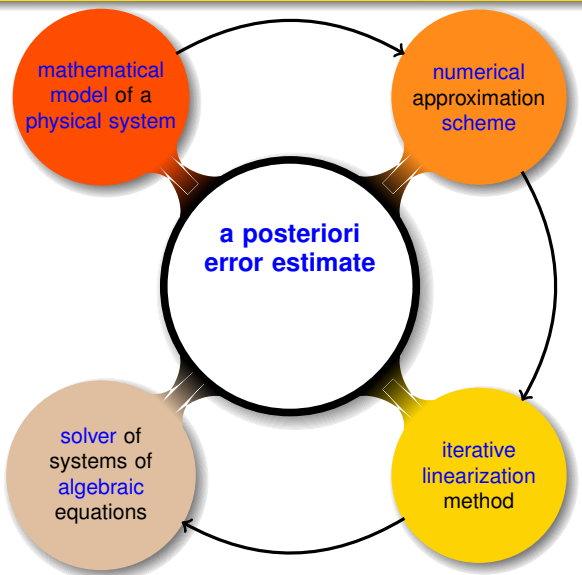
numerical simulation

Control the error and act adaptively: numerical simulations



numerical simulation

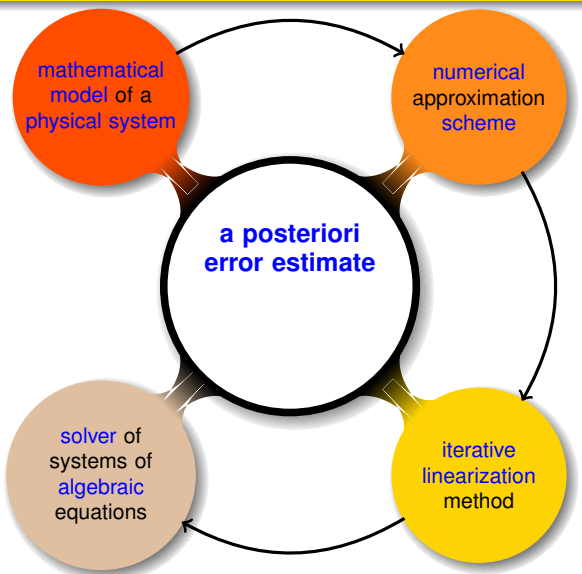
Control the error and act adaptively: numerical simulations



numerical simulation

$\Longleftarrow$ **control the error (a posteriori estimates)**

Control the error and act adaptively: numerical simulations



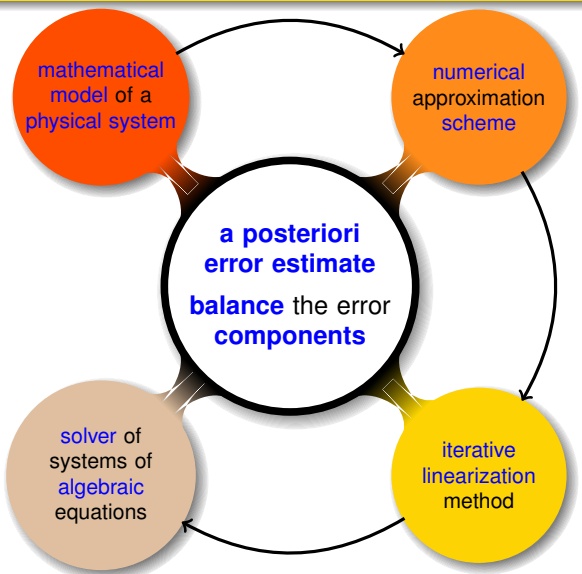
numerical simulation

$\Longleftarrow$ **control the error (a posteriori estimates)**

hard since

- **target unknown**
-

Control the error and act adaptively: numerical simulations



numerical simulation

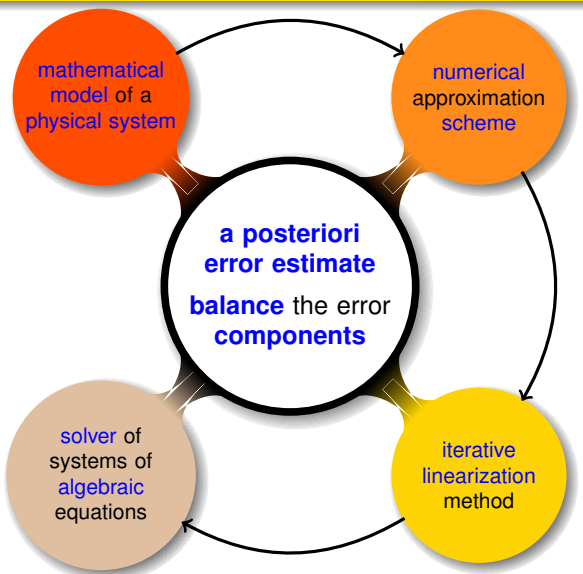
$\Longleftarrow$ **control the error (a posteriori estimates)**

$\Longleftarrow$ **act adaptively (adaptivity)**

hard since

- **target unknown**
-

Control the error and act adaptively: numerical simulations



numerical simulation

$\Longleftarrow$ **control the error (a posteriori estimates)**

$\Longleftarrow$ **act adaptively (adaptivity)**

hard since

- **target unknown**
- **components unknown**

CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

probably **numerical simulations done with insufficient precision**,

Case Studies in Engineering Failure Analysis 3 (2015) 88–95

Contents lists available at ScienceDirect

Case Studies in Engineering Failure Analysis

journal homepage: www.elsevier.com/locate/csefa

Reliability study and simulation of the progressive collapse of Roissy Charles de Gaulle Airport

Y. El Kamari [a], W. Raphael [a,*], A. Chateauneuf [b,c]

[a] École Supérieure d'Ingénieurs de Beyrouth (ESIB), Université Saint-Joseph, CST Mar Roukos, PO Box 11-514, Riad El Solh Beirut 1107 2050, Lebanon

CDG Terminal 2E collapse in 2004 (opened in 2003)



- no earthquake, flooding, tsunami, heavy rain, extreme temperature
- deterministic, steady problem, PDE known, data known, implementation OK

probably **numerical simulations done with insufficient precision**,
I believe **without error control**

Case Studies in Engineering Failure Analysis 3 (2015) 88–95

Contents lists available at ScienceDirect

Case Studies in Engineering Failure Analysis

journal homepage: www.elsevier.com/locate/csefa

Reliability study and simulation of the progressive collapse of Roissy Charles de Gaulle Airport

Y. El Kamari [a], W. Raphael [a,*], A. Chateauneuf [b,c]

[a] École Supérieure d'Ingénieurs de Beyrouth (ESIB), Université Saint-Joseph, CST Mar Roukos, PO Box 11-514, Riad El Solh Beirut 1107 2050, Lebanon

Outline

1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

Numerical approximations of nonlinear PDEs:

Setting

- u: unknown exact PDE solution
- u_ℓ : known numerical approximation on mesh $\mathcal{T}_\ell$



Numerical approximations of nonlinear PDEs:

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Numerical approximations of nonlinear PDEs: **3 crucial questions**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?

Numerical approximations of nonlinear PDEs: **3 crucial questions**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?
2. **Where** (space/linearization/algebra) is it **localized**?

Numerical approximations of nonlinear PDEs: **3 crucial questions**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?
2. **Where** (space/linearization/algebra) is it **localized**?
3. Can we **decrease** it **optimally**?

Numerical approximations of nonlinear PDEs: **3 crucial questions & suggested answers**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?
2. **Where** (space/linearization/algebra) is it **localized**?
3. Can we **decrease** it **optimally**?

Suggested answers

1. Computable **a posteriori** error **estimates**.

Numerical approximations of nonlinear PDEs: **3 crucial questions & suggested answers**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?
2. **Where** (space/linearization/algebra) is it **localized**?
3. Can we **decrease** it **optimally**?

Suggested answers

1. Computable **a posteriori** error **estimates**.
2. Identification of **error components**.

Numerical approximations of nonlinear PDEs: **3 crucial questions & suggested answers**

Setting

- u: unknown exact PDE solution
- $u_\ell^{k,i}$: known numerical approximation on mesh $\mathcal{T}_\ell$, linearization step k, and linear solver step i

Crucial questions

1. How **large** is the overall **error** between u and $u_\ell^{k,i}$?
2. **Where** (space/linearization/algebra) is it **localized**?
3. Can we **decrease** it **optimally**?

Suggested answers

1. Computable **a posteriori** error **estimates**.
2. Identification of **error components**.
3. **Balancing** error components, **adaptivity** (working where needed).

Outline

1. Introduction
   - Textbook numerical approximation and analysis
   - Adaptive numerical approximation and analysis
   - Motivations
   - Crucial questions and answers
   - Achievements and example results
2. Steady nonlinear diffusion
   - A posteriori error estimates (overall and components)
   - Adaptivity of error components: mesh and solvers
3. Multiphase multicompositional flows
   - Error control and adaptivity of error components
4. Conclusions

A posteriori error estimates

A posteriori error estimates

a posteriori error estimates

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i})$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i})$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i}) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**, **robust** with respect to **strength of nonlinearities**

$$|||u - u_\ell^{k,i}||| \leq \eta(u_\ell^{k,i}) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||, \quad C_{\mathrm{eff}} \text{ independent of nonlinearities}$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates **efficient**, **robust** with respect to **strength of nonlinearities**

$$|||u - u_\ell^{k,i}||| \leq \left\{ \sum_{K \in \mathcal{T}_\ell} \eta_K \left(u_\ell^{k,i}\right)^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates, **locally efficient**, **robust** with respect to **strength of nonlinearities**

$$\left\{ \sum_{K\in\mathcal{T}_\ell} \eta_K\big(u_\ell^{k,i}\big)^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

$$\eta_K\big(u_\ell^{k,i}\big) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||_{\omega_K} \text{ for all } K \in \mathcal{T}_\ell,$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates, **locally efficient**, **robust** with respect to **strength of nonlinearities**, and identifying **error components**.

$$\left\{ \sum_{K \in \mathcal{T}_\ell} \eta_K \left(u_\ell^{k,i}\right)^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

$$\eta_K \left(u_\ell^{k,i}\right) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||_{\omega_K} \text{ for all } K \in \mathcal{T}_\ell,$$

$$\eta_K \left(u_\ell^{k,i}\right) = \eta_{\mathrm{disc},K}\left(u_\ell^{k,i}\right) + \eta_{\mathrm{lin},K}\left(u_\ell^{k,i}\right) + \eta_{\mathrm{alg},K}\left(u_\ell^{k,i}\right).$$

A posteriori error estimates

A posteriori error estimates

Guaranteed a posteriori error estimates, **locally efficient**, **robust** with respect to **strength of nonlinearities**, and identifying **error components**.

$$\left\{ \sum_{K\in\mathcal{T}_\ell} \eta_K\left(u_\ell^{k,i}\right)^2 \right\}^{1/2} \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||,$$

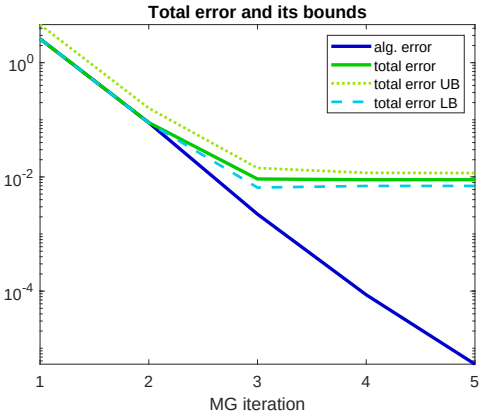
$$\eta_K\left(u_\ell^{k,i}\right) \leq C_{\mathrm{eff}} |||u - u_\ell^{k,i}|||_{\omega_K} \text{ for all } K \in \mathcal{T}_\ell,$$

$$\eta_K\left(u_\ell^{k,i}\right) = \eta_{\mathrm{disc},K}\left(u_\ell^{k,i}\right) + \eta_{\mathrm{lin},K}\left(u_\ell^{k,i}\right) + \eta_{\mathrm{alg},K}\left(u_\ell^{k,i}\right).$$

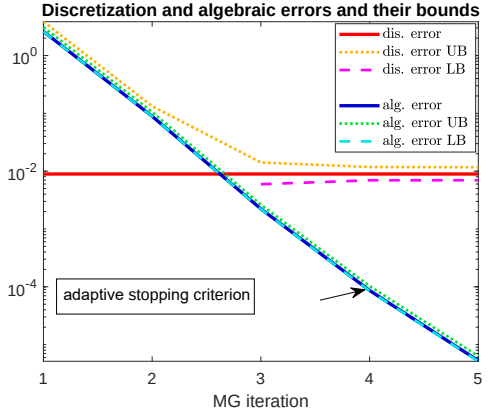
Error components

- $\eta_{\mathrm{disc},K}\left(u_\ell^{k,i}\right)$: discretization
- $\eta_{\mathrm{lin},K}\left(u_\ell^{k,i}\right)$: linearization
- $\eta_{\mathrm{alg},K}\left(u_\ell^{k,i}\right)$: algebraic solver

A posteriori estimates of **total** and **algebraic errors**: $\mathbb{A}_\ell \mathrm{U}_\ell^j \neq \mathrm{F}_\ell$



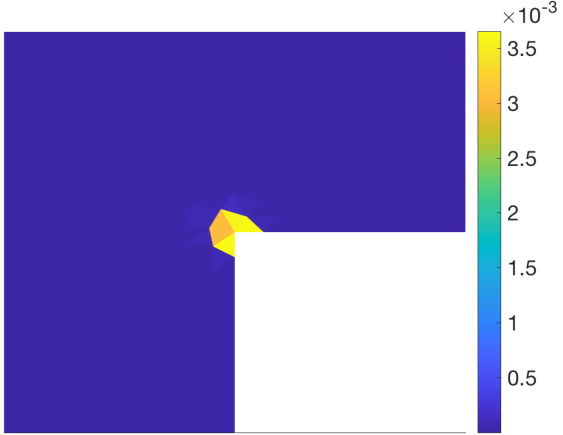
Total error



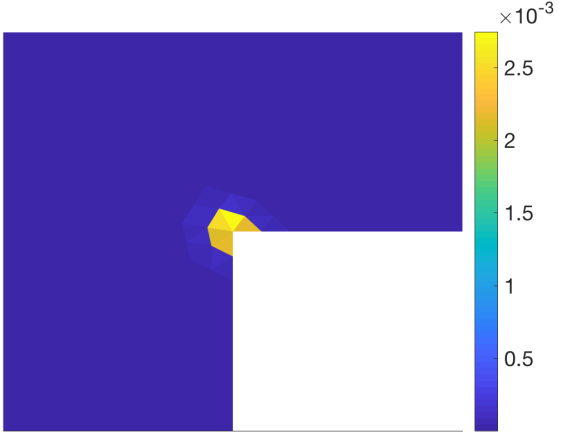
Error components and adaptive st. crit.

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

A posteriori estimates of **total** and **algebraic errors**: $\mathbb{A}_\ell \mathbf{U}_\ell^i \neq \mathbf{F}_\ell$



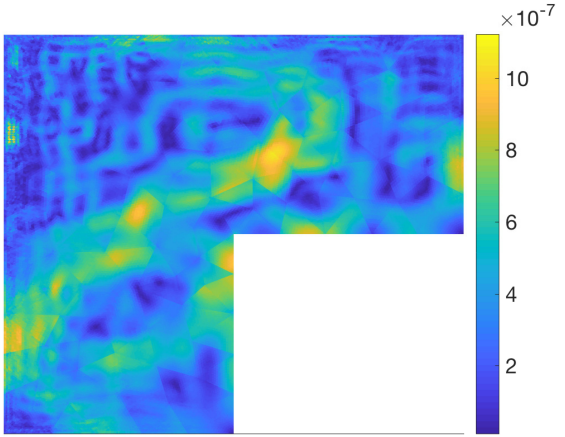
Estimated total errors $\eta_K(u_\ell^i)$



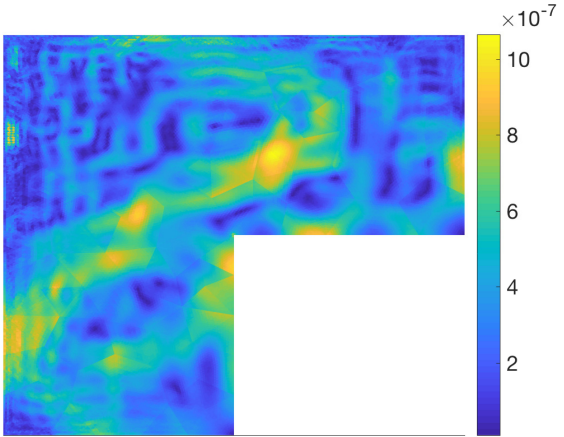
Exact total errors $\|\nabla(u - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

A posteriori estimates of **total** and **algebraic errors**: $\mathbb{A}_\ell \mathbf{U}_\ell^i \neq \mathbf{F}_\ell$



Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Algorithm

Algorithm 1 Adaptivity of error components

while $\frac{\eta(u_\ell^{k,i})}{|||u_\ell^{k,i}|||} > \gamma_{\text{tot}}$ **do** ▷ while user-specified relative precision is not reached

  assemble the finite element space V_ℓ^p

  assemble the nonlinear problem

  while $\eta_{\text{lin},K}(u_\ell^{k,i}) > \gamma_{\text{lin}}\eta_{\text{disc},K}(u_\ell^{k,i})$ $\forall K \in \mathcal{T}_\ell$ **do** ▷ while linearization dominates discretization

    assemble the linearized problem

    while $\eta_{\text{alg},K}(u_\ell^{k,i}) > \gamma_{\text{alg}}\eta_{\text{lin},K}(u_\ell^{k,i})$ $\forall K \in \mathcal{T}_\ell$ **do** ▷ while algebra dominates linearization

      one step of iterative algebraic solver, $i++$

    end while (iterative algebraic solver)

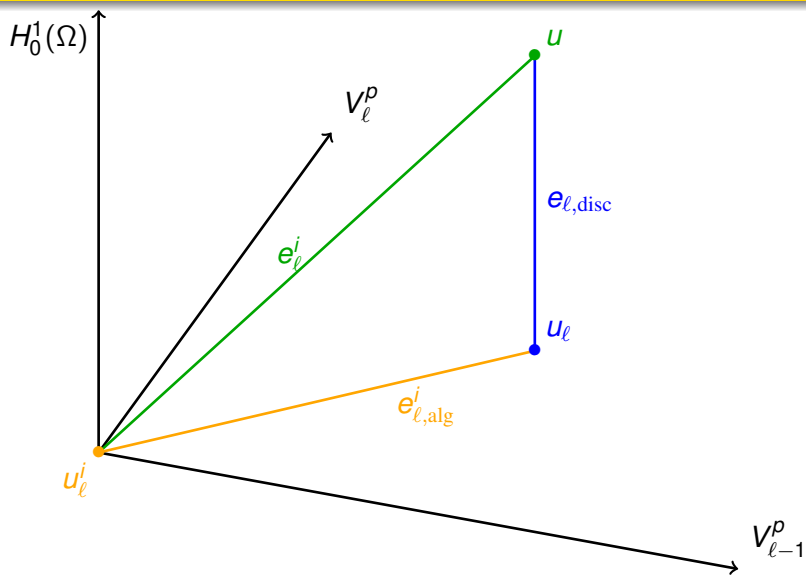
    $k++$

  end while (iterative linearization)

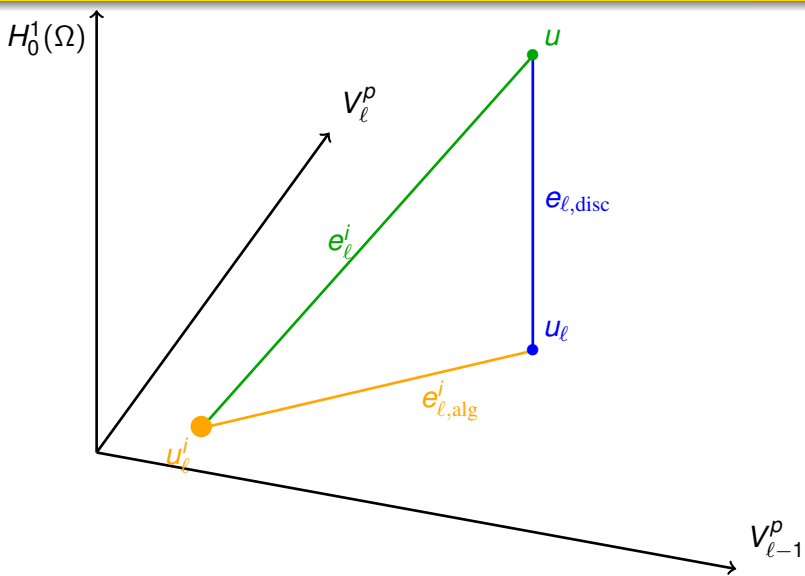
  refine $K \in \mathcal{T}_\ell$ with big $\eta_{\text{disc},K}(u_\ell^{k,i})$, $\ell++$

end while (adaptive mesh refinement)

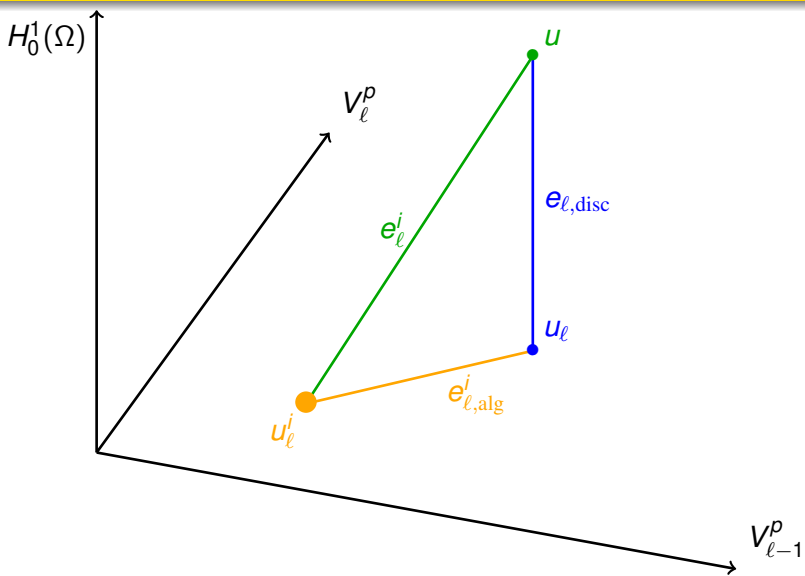
Algorithm


$H_0^1(\Omega)$
u
V_ℓ^p
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$V_{\ell-1}^p$

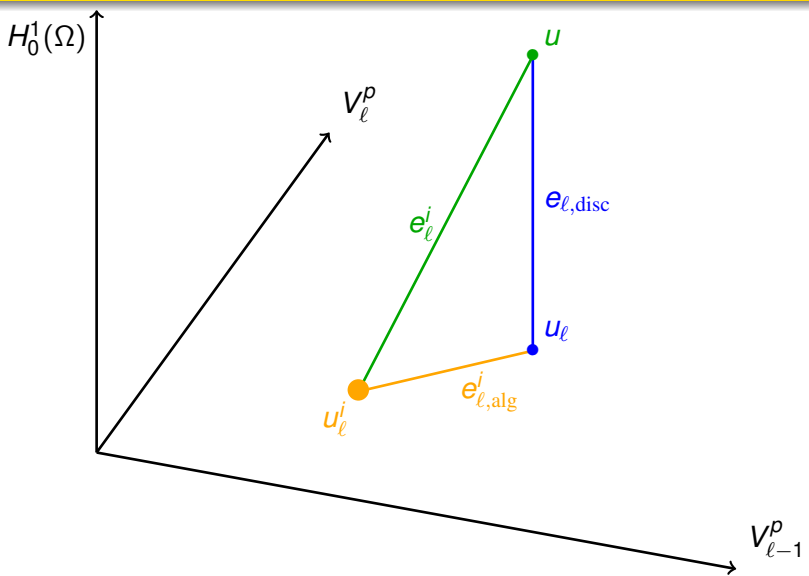
Algorithm


$H_0^1(\Omega)$
u
V_ℓ^p
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$V_{\ell-1}^p$

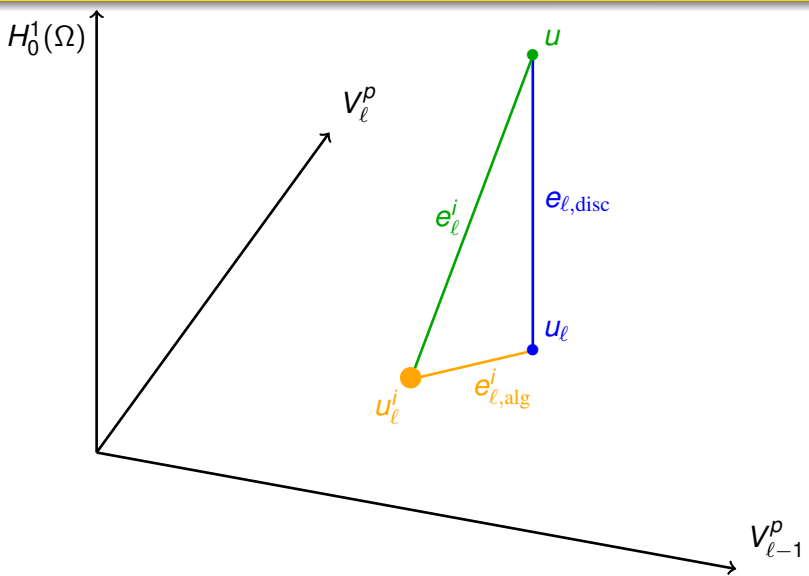
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$V_{\ell-1}^p$

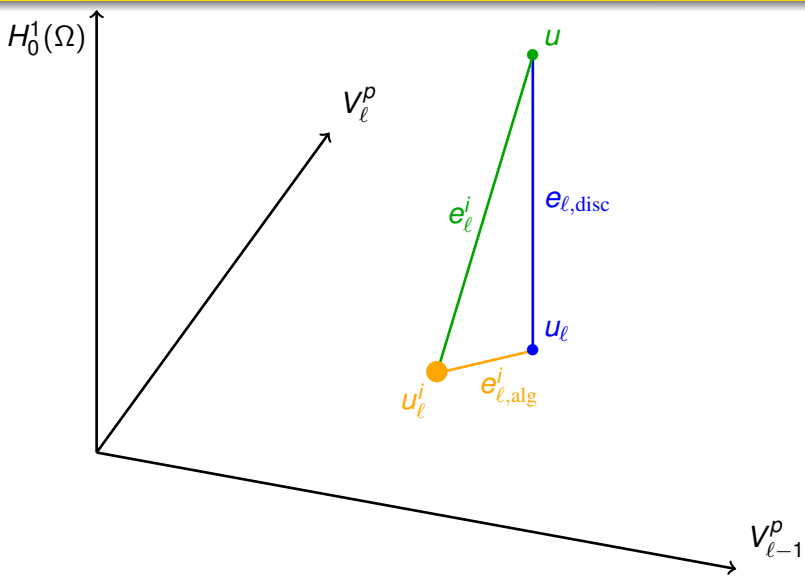
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$V_{\ell-1}^p$

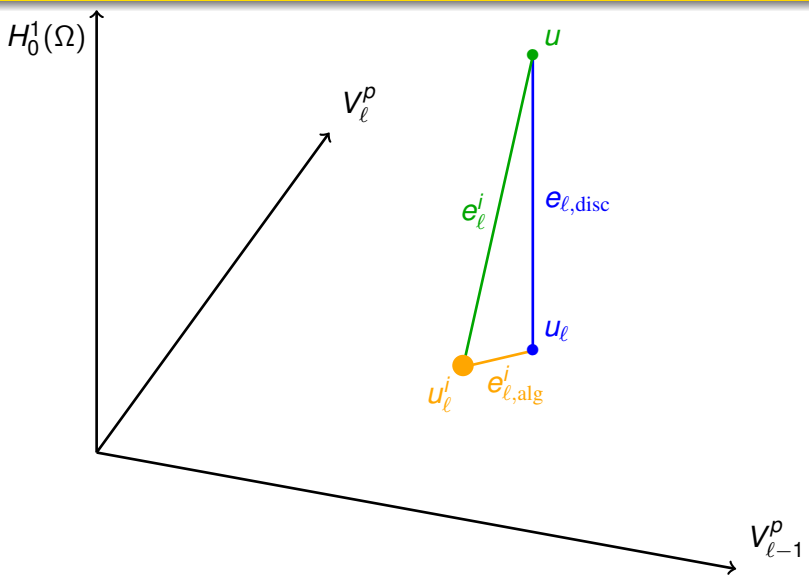
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
e_ℓ^i
$e_{\ell,\mathrm{disc}}$
u_ℓ
u_ℓ^i
$e_{\ell,\mathrm{alg}}^i$
$V_{\ell-1}^p$

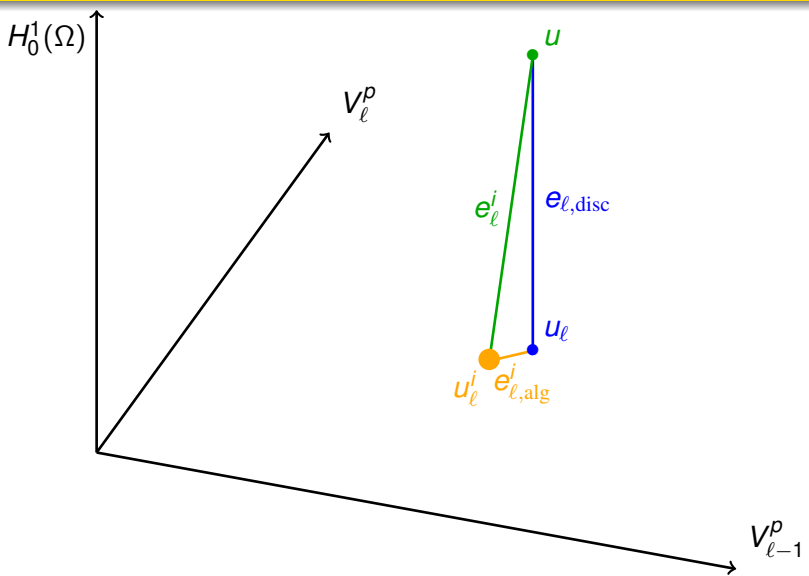
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
e_ℓ^i
$e_{\ell,\mathrm{disc}}$
u_ℓ
u_ℓ^i
$e_{\ell,\mathrm{alg}}^i$
$V_{\ell-1}^p$

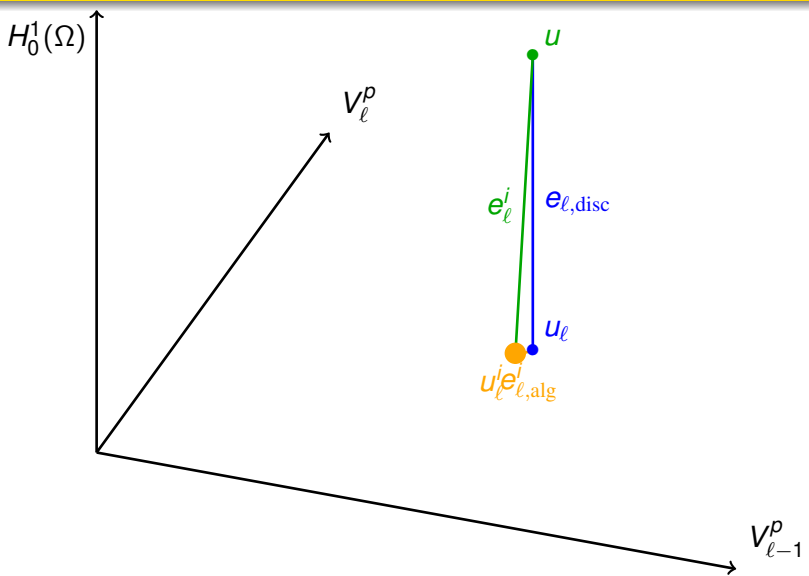
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
e_ℓ^i
$e_{\ell,\mathrm{disc}}$
u_ℓ
u_ℓ^i
$e_{\ell,\mathrm{alg}}^i$
$V_{\ell-1}^p$

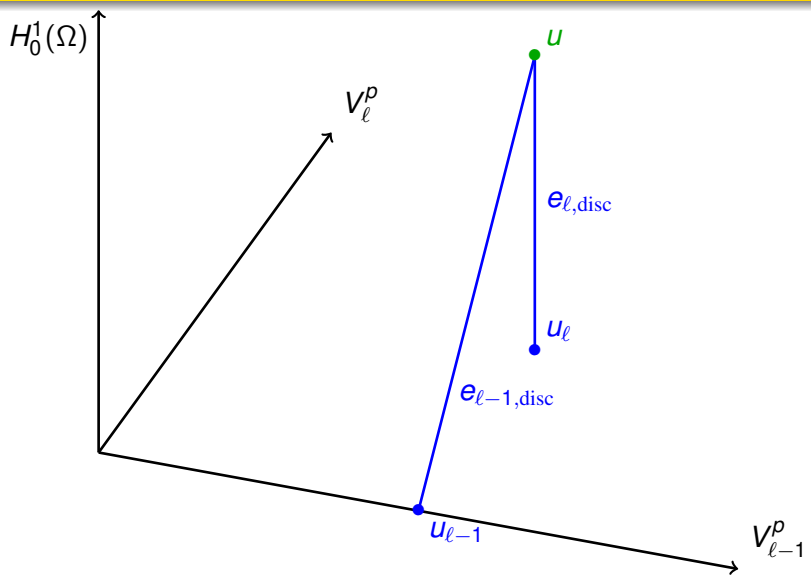
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
e_ℓ^i
$e_{\ell,\mathrm{disc}}$
u_ℓ
u_ℓ^i
$e_{\ell,\mathrm{alg}}^i$
$V_{\ell-1}^p$

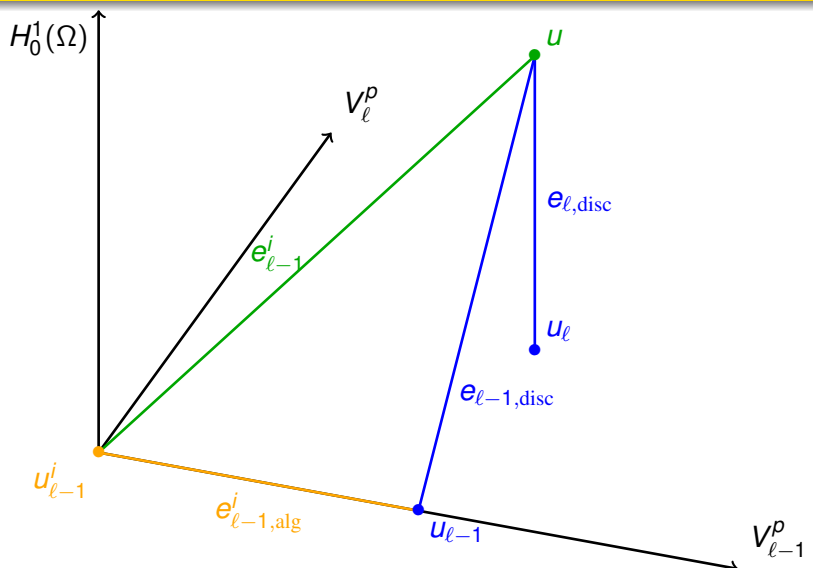
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
e_ℓ^i
$e_{\ell,\mathrm{disc}}$
u_ℓ
u_ℓ^i
$e_{\ell,\mathrm{alg}}^i$
$V_{\ell-1}^p$

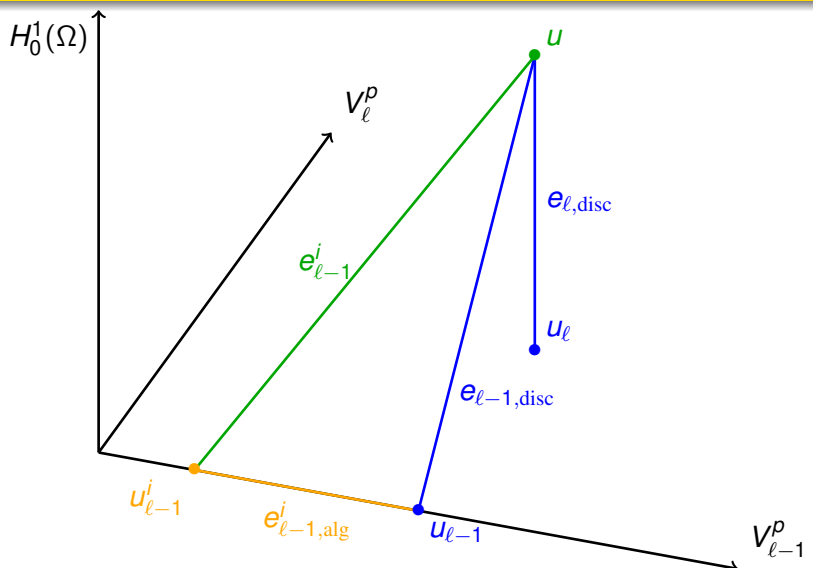
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
u_ℓ
$e_{\ell-1,\mathrm{disc}}$
$u_{\ell-1}$
$V_{\ell-1}^p$

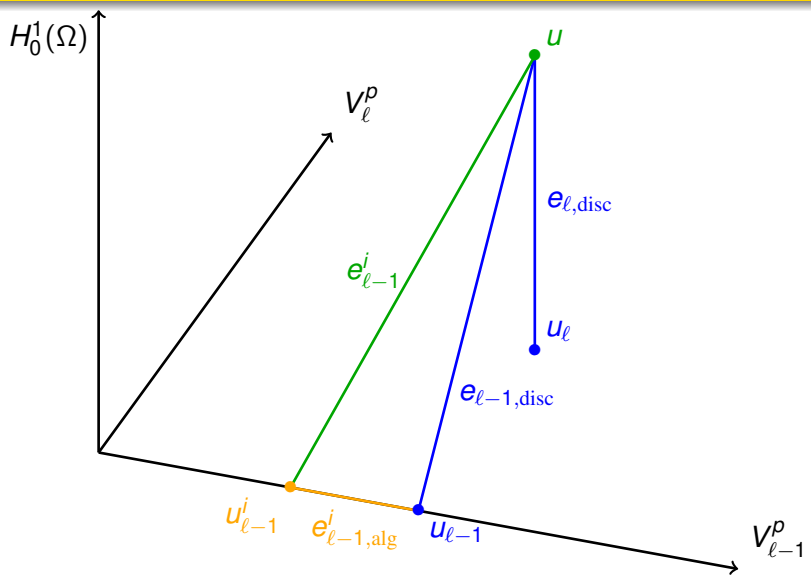
Algorithm


$H_0^1(\Omega)$
u
V_ℓ^p
$e_{\ell,\mathrm{disc}}$
$e_{\ell-1}^i$
u_ℓ
$e_{\ell-1,\mathrm{disc}}$
$u_{\ell-1}^i$
$e_{\ell-1,\mathrm{alg}}^i$
$u_{\ell-1}$
$V_{\ell-1}^p$

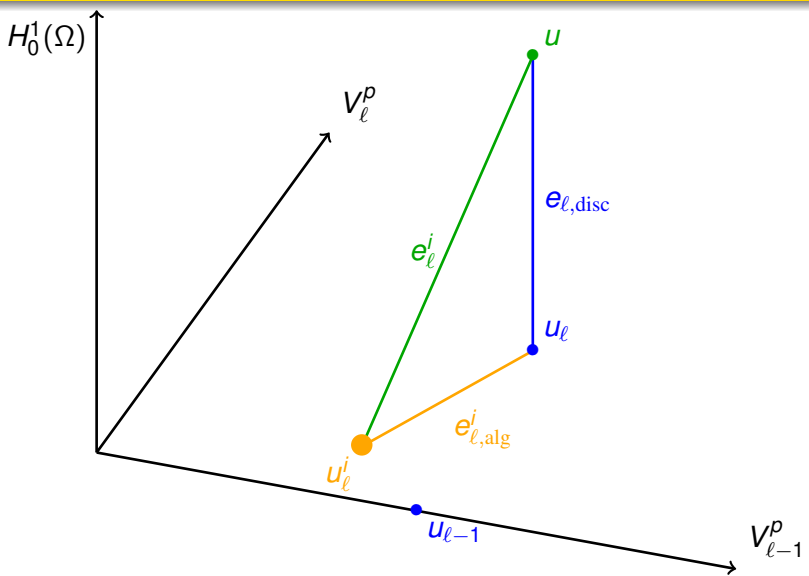
Algorithm


$H_0^1(\Omega)$
u
V_ℓ^p
$e_{\ell,\mathrm{disc}}$
$e_{\ell-1}^i$
u_ℓ
$e_{\ell-1,\mathrm{disc}}$
$u_{\ell-1}^i$
$e_{\ell-1,\mathrm{alg}}^i$
$u_{\ell-1}$
$V_{\ell-1}^p$

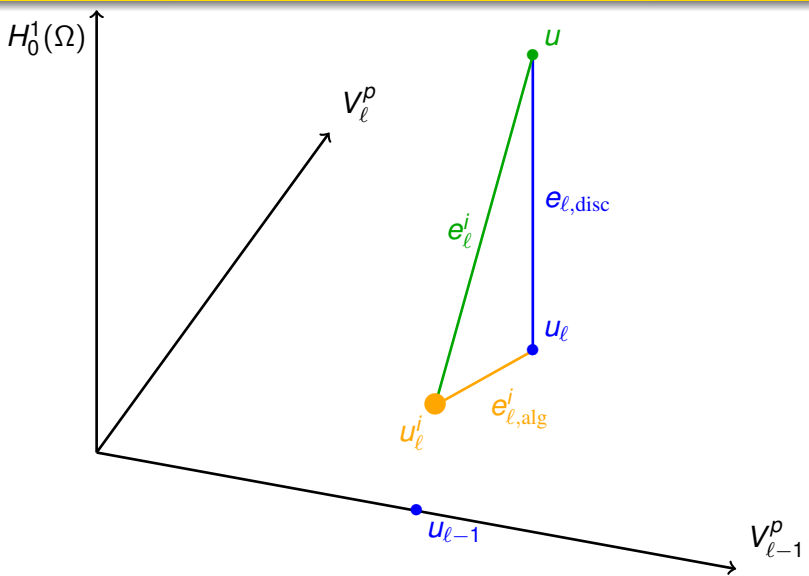
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
$e_{\ell-1}^i$
u_ℓ
$e_{\ell-1,\mathrm{disc}}$
$u_{\ell-1}^i$
$e_{\ell-1,\mathrm{alg}}^i$
$u_{\ell-1}$
$V_{\ell-1}^p$

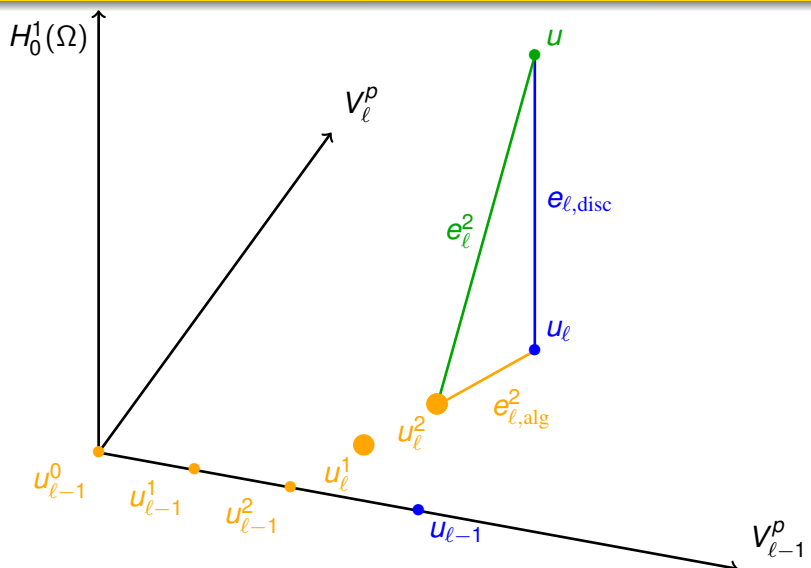
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$u_{\ell-1}$
$V_{\ell-1}^p$

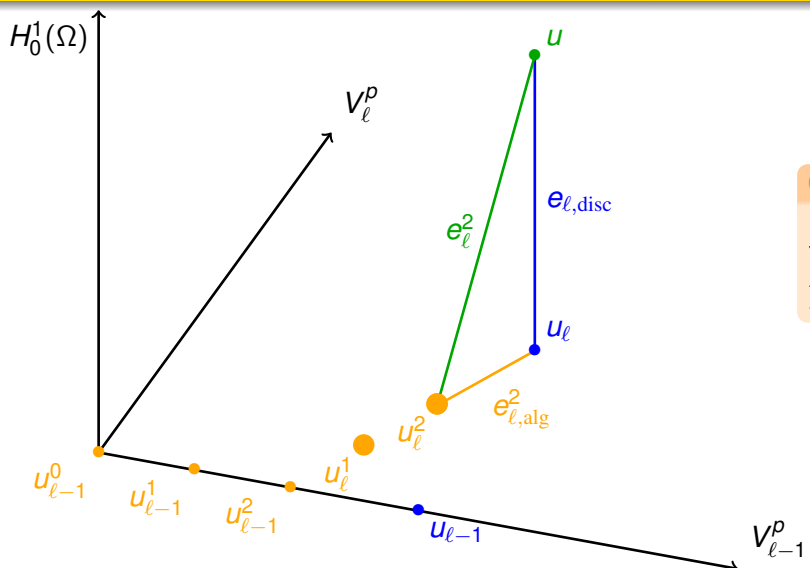
Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
e_ℓ^i
u_ℓ
$e_{\ell,\mathrm{alg}}^i$
u_ℓ^i
$u_{\ell-1}$
$V_{\ell-1}^p$

Algorithm


$H_0^1(\Omega)$
V_ℓ^p
u
$e_{\ell,\mathrm{disc}}$
e_ℓ^2
u_ℓ
$e_{\ell,\mathrm{alg}}^2$
u_ℓ^2
u_ℓ^1
$u_{\ell-1}^0$
$u_{\ell-1}^1$
$u_{\ell-1}^2$
$u_{\ell-1}$
$V_{\ell-1}^p$

Algorithm



Cost

$$\sum_{\ell=0}^{\bar{\ell}} \sum_{i=0}^{\bar{i}} |V_\ell^p|$$

Holistic approach: interplay PDE–numerics–linearization–algebra

Optimal decay rate of error wrt computational cost

Adaptivity of error components allows to achieve

$$|||u - u_{\bar{\ell}}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_\ell^p| \right\}^{-p/d}$$ (replaces traditional a priori h^p).

Holistic approach: interplay PDE–numerics–linearization–algebra

Optimal decay rate of error wrt computational cost

Adaptivity of error components allows to achieve

$$|||u - u_{\bar{\ell}}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_\ell^p| \right\}^{-p/d}$$ (replaces traditional a priori h^p).

Error control

- at **any moment** during the simulation
- price: local finite element quadrature/sparse **matrix-vector** multiplication

Holistic approach: interplay PDE–numerics–linearization–algebra

Optimal decay rate of error wrt computational cost

Adaptivity of error components allows to achieve

$$|||u - u_{\bar{\ell}}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_\ell^p| \right\}^{-p/d}$$ (replaces traditional a priori h^p).

Error control

- at **any moment** during the simulation
- price: local finite element quadrature/sparse **matrix-vector** multiplication

Adaptivity of error components

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering** (work where needed)

Holistic approach: interplay PDE–numerics–linearization–algebra

Optimal decay rate of error wrt computational cost

Adaptivity of error components allows to achieve

$$|||u - u_{\ell}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_{\ell}^{p}| \right\}^{-p/d} \quad \text{(replaces traditional a priori } h^{p}\text{)}.$$

Error control

- at **any moment** during the simulation
- price: local finite element quadrature/sparse **matrix-vector** multiplication

Adaptivity of error components

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering** (work where needed)
- hard problem replaced by a **sequence** of **easier problems**

Holistic approach: interplay PDE–numerics–linearization–algebra

Optimal decay rate of error wrt computational cost

Adaptivity of error components allows to achieve

$$|||u - u_{\bar{\ell}}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_\ell^p| \right\}^{-p/d} \quad \text{(replaces traditional a priori } h^p\text{)}.$$

Error control

- at **any moment** during the simulation
- price: local finite element quadrature/sparse **matrix-vector** multiplication

Adaptivity of error components

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering** (work where needed)
- hard problem replaced by a **sequence** of **easier problems**
- not a novel scheme, rather an **efficient use** of existing **building blocks**



Outline

1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions

A model nonlinear problem

Find $u \in H_0^1(\Omega)$ such that

$$\underbrace{\left(a(|\nabla u|)\nabla u, \nabla v\right)}_{\langle \mathcal{A}(u), v\rangle\text{: nonlinear operator}} = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

A model nonlinear problem

Find $u \in H_0^1(\Omega)$ such that

$$\underbrace{(a(|\nabla u|)\nabla u, \nabla v)}_{\langle \mathcal{A}(u), v\rangle\text{: nonlinear operator}} = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

Assumption (Gradient-dependent diffusivity)

Function $a : [0,\infty) \to (0,\infty)$, *for all* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$,

$$|a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}| \le a_c|\boldsymbol{x} - \boldsymbol{y}| \qquad \textit{(Lipschitz continuity)},$$
$$(a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}) \cdot (\boldsymbol{x} - \boldsymbol{y}) \ge a_m|\boldsymbol{x} - \boldsymbol{y}|^2 \qquad \textit{(strong monotonicity)}.$$

A model nonlinear problem

Find $u \in H_0^1(\Omega)$ such that

$$\underbrace{(a(|\nabla u|)\nabla u, \nabla v)}_{\langle \mathcal{A}(u), v\rangle\text{: nonlinear operator}} = (f, v) \qquad \forall v \in H_0^1(\Omega).$$

Assumption (Gradient-dependent diffusivity)

Function $a : [0,\infty) \to (0,\infty)$, *for all* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$,

$$|a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}| \le a_c|\boldsymbol{x}-\boldsymbol{y}| \qquad \textit{(Lipschitz continuity)},$$
$$(a(|\boldsymbol{x}|)\boldsymbol{x} - a(|\boldsymbol{y}|)\boldsymbol{y}) \cdot (\boldsymbol{x}-\boldsymbol{y}) \ge a_m|\boldsymbol{x}-\boldsymbol{y}|^2 \qquad \textit{(strong monotonicity)}.$$

- $a_m \le a(r) \le a_c$, $a_m \le (a(r)r)' \le a_c$

Example of the nonlinear function a

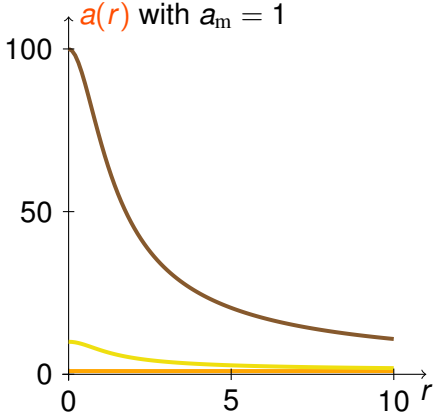
Example (Mean curvature nonlinearity)

$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$

Example of the nonlinear function a

Example (Mean curvature nonlinearity)

$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$

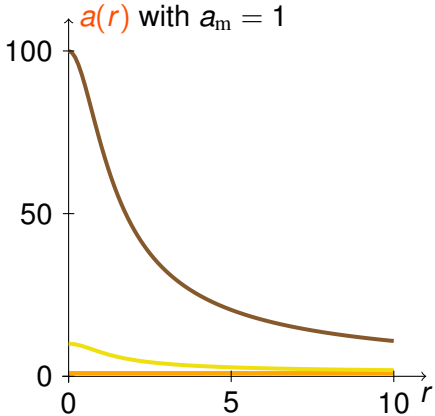


$a_{\mathrm{c}} = 100$
$a_{\mathrm{c}} = 10$
$a_{\mathrm{c}} = 1$

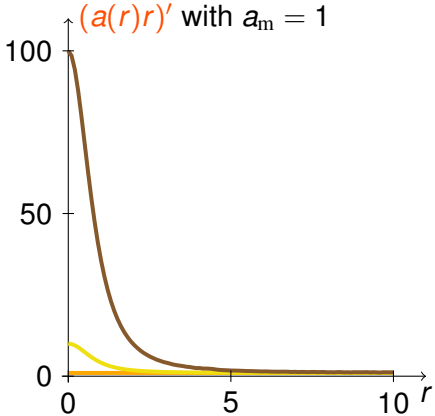
Example of the nonlinear function a

Example (Mean curvature nonlinearity)

$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$



$a_{\mathrm{c}} = 100$
$a_{\mathrm{c}} = 10$
$a_{\mathrm{c}} = 1$



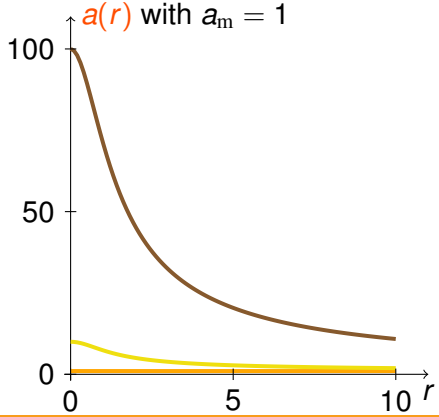
Example of the nonlinear function a

Example (Mean curvature nonlinearity)

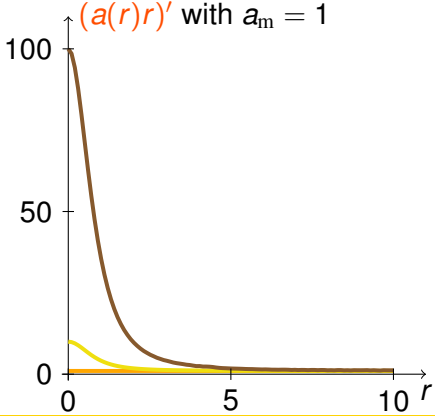
$$a(r) := a_{\mathrm{m}} + \frac{a_{\mathrm{c}} - a_{\mathrm{m}}}{\sqrt{1 + r^2}}.$$

Strength of the nonlinearity

$$\frac{a_{\mathrm{c}}}{a_{\mathrm{m}}} = \frac{\text{Lipschitz continuity}}{\text{strong monotonicity}}$$



$a_{\mathrm{c}} = 100$
$a_{\mathrm{c}} = 10$
$a_{\mathrm{c}} = 1$



Finite element discretization

Definition (Finite element discretization)

Find $u_\ell \in V_\ell^p$ such that

$$\underbrace{\left(a(|\nabla u_\ell|)\nabla u_\ell, \nabla v_\ell\right)}_{\langle \mathcal{A}(u_\ell), v_\ell\rangle\text{: nonlinear operator}} = \left(f, v_\ell\right) \qquad \forall v_\ell \in V_\ell^p.$$

Finite element discretization

Definition (Finite element discretization)

Find $u_\ell \in V_\ell^p$ such that

$$\underbrace{\big(a(|\nabla u_\ell|)\nabla u_\ell, \nabla v_\ell\big)}_{\langle \mathcal{A}(u_\ell), v_\ell\rangle\text{: nonlinear operator}} = \big(f, v_\ell\big) \qquad \forall v_\ell \in V_\ell^p.$$

- $\mathcal{T}_\ell$ simplicial mesh of Ω
- $p \geq 1$ polynomial degree
- $V_\ell^p := \mathcal{P}_p(\mathcal{T}_\ell) \cap H_0^1(\Omega)$
- conforming finite elements

Finite element discretization

Definition (Finite element discretization)

Find $u_\ell \in V_\ell^p$ such that

$$\underbrace{\big(a(|\nabla u_\ell|)\nabla u_\ell, \nabla v_\ell\big)}_{\langle \mathcal{A}(u_\ell), v_\ell\rangle\text{: nonlinear operator}} = \big(f, v_\ell\big) \qquad \forall v_\ell \in V_\ell^p.$$

- $\mathcal{T}_\ell$ simplicial mesh of Ω
- $p \geq 1$ polynomial degree
- $V_\ell^p := \mathcal{P}_p(\mathcal{T}_\ell) \cap H_0^1(\Omega)$
- conforming finite elements
- system of **nonlinear algebraic equations**

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}
- $u_\ell^0 := u_{\ell-1}^{\overline{k},\bar{i}} \in V_\ell^p$ initial guess from the previous mesh

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}
- $u_\ell^0 := u_{\ell-1}^{\overline{k},\bar{i}} \in V_\ell^p$ initial guess from the previous mesh
- system of **linear algebraic equations**

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}
- $u_\ell^0 := u_{\ell-1}^{\overline{k},\bar{i}} \in V_\ell^p$ initial guess from the previous mesh
- system of **linear algebraic equations**
- examples
  - $\boldsymbol{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\boldsymbol{I}_d$, $\boldsymbol{b}_\ell^{k-1} = \boldsymbol{0}$ (fixed-point/Picard)

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}
- $u_\ell^0 := u_{\ell-1}^{\overline{k},\bar{i}} \in V_\ell^p$ initial guess from the previous mesh
- system of **linear algebraic equations**
- examples
  - $\boldsymbol{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\boldsymbol{I}_d$, $\boldsymbol{b}_\ell^{k-1} = \boldsymbol{0}$ (fixed-point/Picard)
  - $\boldsymbol{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\boldsymbol{I}_d + \frac{a'(|\nabla u_\ell^{k-1}|)}{|\nabla u_\ell^{k-1}|}\nabla u_\ell^{k-1} \otimes \nabla u_\ell^{k-1}$,
    $\boldsymbol{b}_\ell^{k-1} = a'(|\nabla u_\ell^{k-1}|)|\nabla u_\ell^{k-1}|\nabla u_\ell^{k-1}$ (Newton)

Iterative linearization

Definition (Linearized finite element approximation)

Find $u_\ell^k \in V_\ell^p$ such that

$$\underbrace{(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^k - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell)}_{\langle \mathcal{A}^{k-1}(u_\ell^k), v_\ell\rangle\text{: linearized operator}} = (f, v_\ell) \qquad \forall v_\ell \in V_\ell^p.$$

- iterative linearization index $k \geq 1$
- $\boldsymbol{A}_\ell^{k-1}$, $\boldsymbol{b}_\ell^{k-1}$: matrix- and vector-valued functions constructed from u_ℓ^{k-1}
- $u_\ell^0 := u_{\ell-1}^{\overline{k},\overline{i}} \in V_\ell^p$ initial guess from the previous mesh
- system of **linear algebraic equations**
- examples
  - $\boldsymbol{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\boldsymbol{I}_d$, $\boldsymbol{b}_\ell^{k-1} = \boldsymbol{0}$ (fixed-point/Picard)
  - $\boldsymbol{A}_\ell^{k-1} = a(|\nabla u_\ell^{k-1}|)\boldsymbol{I}_d + \frac{a'(|\nabla u_\ell^{k-1}|)}{|\nabla u_\ell^{k-1}|}\nabla u_\ell^{k-1} \otimes \nabla u_\ell^{k-1}$,
    $\boldsymbol{b}_\ell^{k-1} = a'(|\nabla u_\ell^{k-1}|)|\nabla u_\ell^{k-1}|\nabla u_\ell^{k-1}$ (Newton)
  - $\boldsymbol{A}_\ell^{k-1} = \gamma \boldsymbol{I}_d$ with $\gamma \geq \frac{a_c^2}{a_m}$, $\boldsymbol{b}_\ell^{k-1} = (\gamma - a(|\nabla u_\ell^{k-1}|))\nabla u_\ell^{k-1}$ (Zarantonello)

Iterative algebraic solver

Definition (Iterative algebraic solver)

Find $u_\ell^{k,i} \in V_\ell^p$ such that

$$(\boldsymbol{A}_\ell^{k-1} \nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) = (f, v_\ell) - \underbrace{(r_\ell^{k,i}, v_\ell)}_{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v_\ell \rangle\text{: algebraic residual}} \qquad \forall v_\ell \in V_\ell^p.$$

Iterative algebraic solver

Definition (Iterative algebraic solver)

Find $u_\ell^{k,i} \in V_\ell^p$ such that

$$(\boldsymbol{A}_\ell^{k-1} \nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) = (f, v_\ell) - \underbrace{(r_\ell^{k,i}, v_\ell)}_{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v_\ell \rangle\text{: algebraic residual}} \qquad \forall v_\ell \in V_\ell^p.$$

- iterative algebraic solver index $i \geq 1$

Iterative algebraic solver

Definition (Iterative algebraic solver)

Find $u_\ell^{k,i} \in V_\ell^p$ such that

$$(\boldsymbol{A}_\ell^{k-1} \nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) = (f, v_\ell) - \underbrace{(r_\ell^{k,i}, v_\ell)}_{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v_\ell \rangle\text{: algebraic residual}} \qquad \forall v_\ell \in V_\ell^p.$$

- iterative algebraic solver index $i \geq 1$
- $u_\ell^{k,0} := u_\ell^{k-1,\bar{i}} \in V_\ell^p$ initial guess from the previous linearization step

Iterative algebraic solver

Definition (Iterative algebraic solver)

Find $u_\ell^{k,i} \in V_\ell^p$ such that

$$(\boldsymbol{A}_\ell^{k-1} \nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}, \nabla v_\ell) = (f, v_\ell) - \underbrace{(r_\ell^{k,i}, v_\ell)}_{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v_\ell \rangle\text{: algebraic residual}} \qquad \forall v_\ell \in V_\ell^p.$$

- iterative algebraic solver index $i \geq 1$
- $u_\ell^{k,0} := u_\ell^{k-1,\bar{i}} \in V_\ell^p$ initial guess from the previous linearization step
- algebraic residual: discrete, known

Outline

1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions

Error measure, error components

Definition (Intrinsic measure of error)

$$|||u - u_\ell^{k,i}||| := \max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\| = 1}} \{ \underbrace{(f, v) - (a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i}, \nabla v)}_{} \}$$

Error measure, error components

Definition (Intrinsic measure of error)

$$|||u - u_\ell^{k,i}||| := \max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \{ \underbrace{(f,v) - (a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i}, \nabla v)}_{\langle \mathcal{R}(u_\ell^{k,i}), v\rangle\text{: total residual}} \}$$

Error measure, error components

Definition (Intrinsic measure of error)

$$|||u - u_\ell^{k,i}||| := \max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \{ \underbrace{(f,v) - (a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i}, \nabla v)}_{\langle \mathcal{R}(u_\ell^{k,i}), v\rangle\text{: total residual}=(f,v)-\langle \mathcal{A}(u_\ell^{k,i}), v\rangle} \}$$

Error measure, error components

Definition (Intrinsic measure of error)

$$|||u - u_\ell^{k,i}||| := \max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \{ \underbrace{(f,v) - (a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i}, \nabla v)}_{\langle \mathcal{R}(u_\ell^{k,i}),v\rangle\text{: total residual}=(f,v)-\langle \mathcal{A}(u_\ell^{k,i}),v\rangle} \}$$

Error components

$$\underbrace{(f,v) - \langle \mathcal{A}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}(u_\ell^{k,i}),v\rangle\text{: total residual}} = \underbrace{(f,v) - \langle \mathcal{A}^{k-1}(u_\ell^{k,i}), v\rangle - \langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}^{\mathrm{disc}}(u_\ell^{k,i}),v\rangle\text{: discretization residual}}$$
$$+ \underbrace{\langle \mathcal{A}^{k-1}(u_\ell^{k,i}), v\rangle - \langle \mathcal{A}(u_\ell^{k,i}), v\rangle}_{\langle \mathcal{R}^{\mathrm{lin}}(u_\ell^{k,i}),v\rangle\text{: linearization residual}}$$
$$+ \underbrace{\langle \mathcal{R}^{\mathrm{alg}}(u_\ell^{k,i}), v\rangle}_{\text{algebraic residual}}$$

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the PDE residual}} .$$

$$= \min_{\substack{v \in H(\mathrm{div},\Omega) \\ \nabla \cdot v = f}} \|\nabla u_\ell + v\|^2$$

constrained distance to $H(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\sigma_\ell \in H(\mathrm{div},\Omega)$ with $\nabla \cdot \sigma_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \leq \|\nabla u_\ell + \sigma_\ell\|$.

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H^1_0(\Omega)$ be the weak solution and let $u_\ell \in H^1_0(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H^1_0(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the PDE residual}} .$$

$$= \min_{\substack{v \in H(\mathrm{div},\Omega) \\ \nabla \cdot v = f}} \|\nabla u_\ell + v\|^2$$

constrained distance to $H(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\sigma_\ell \in H(\mathrm{div},\Omega)$ with $\nabla \cdot \sigma_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \le \|\nabla u_\ell + \sigma_\ell\|$.

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the PDE residual}} = \min_{\substack{\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div},\Omega) \\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_\ell + \boldsymbol{v}\|^2$$

constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div},\Omega)$ with $\nabla\cdot\boldsymbol{\sigma}_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \le \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|$.

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the PDE residual}} = \min_{\substack{\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div},\Omega) \\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_\ell + \boldsymbol{v}\|^2$$

constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div}, \Omega)$ with $\nabla\cdot\boldsymbol{\sigma}_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \le \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|$.
- Local contributions by Ladevèze (1975), Ladevèze & Pelle (1983), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Mercier & Pilkington & Scholberg (2010), Kim & Kwak (2010), Braess & Pillwein & Schöberl (2010), Repin & Valdman (2016), ...

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the } \textbf{PDE residual}} .$$

$$= \min_{\substack{\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div},\Omega) \\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_\ell + \boldsymbol{v}\|^2$$

constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div}, \Omega)$ with $\nabla\cdot\boldsymbol{\sigma}_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \leq \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|$.
- Local construction of $\boldsymbol{\sigma}_\ell$: Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Vejchodský (2006), Braess, Pillwein, & Schöberl (2008), Ern & Vohralík (2013)

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947))

Let $u \in H_0^1(\Omega)$ be the weak solution and let $u_\ell \in H_0^1(\Omega)$ be arbitrary. Then

$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H_0^1(\Omega) \\ \|\nabla v\|=1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the PDE residual}} = \min_{\substack{\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div},\Omega) \\ \nabla\cdot\boldsymbol{v}=f}} \|\nabla u_\ell + \boldsymbol{v}\|^2$$

constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

Comments

- It is enough to choose suitable (discrete, piecewise polynomial) $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div}, \Omega)$ with $\nabla\cdot\boldsymbol{\sigma}_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \leq \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|$.
- **Local** construction of σ_ℓ: Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Vejchodský (2006), Braess, Pillwein, & Schöberl (2008), Ern & Vohralík (2013)

Duality when $a = 1$ (linear case)

Theorem (Error characterization, Prager & Synge (1947)**)**

Let $u \in H^1_0(\Omega)$ be the weak solution and let $u_\ell \in H^1_0(\Omega)$ be arbitrary. Then

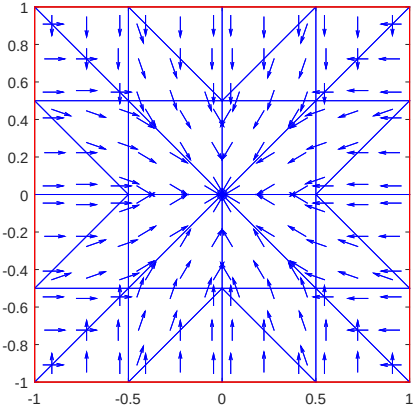
$$\|\nabla(u - u_\ell)\|^2 = \underbrace{\max_{\substack{v \in H^1_0(\Omega) \\ \|\nabla v\| = 1}} \underbrace{\{(f, v) - (\nabla u_\ell, \nabla v)\}^2}_{\langle \mathcal{R}(u_\ell), v \rangle}}_{\text{dual norm of the } \textbf{PDE residual}} = \min_{\substack{\boldsymbol{v} \in \boldsymbol{H}(\mathrm{div},\Omega) \\ \nabla \cdot \boldsymbol{v} = f}} \|\nabla u_\ell + \boldsymbol{v}\|^2 .$$

constrained distance to $\boldsymbol{H}(\mathrm{div},\Omega)$

Comments

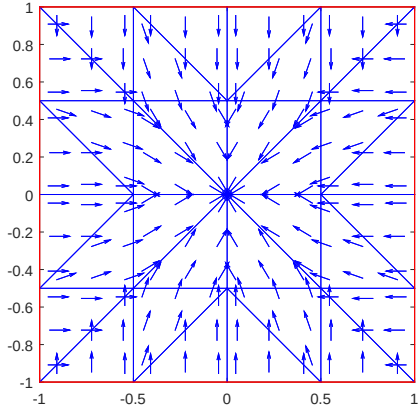
- It is enough to choose suitable (discrete, piecewise polynomial) $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div}, \Omega)$ with $\nabla \cdot \boldsymbol{\sigma}_\ell = f$ to get the guaranteed upper bound $\|\nabla(u - u_\ell)\| \leq \|\nabla u_\ell + \boldsymbol{\sigma}_\ell\|$.
- **Local** construction of $\boldsymbol{\sigma}_\ell$: Ladevèze (1975), Babuška & Rheinboldt (1987), Verfürth (1989), Ainsworth & Oden (1993), Destuynder & Métivet (1999), Vejchodský (2006), Braess, Pillwein, & Schöberl (2008), Ern & Vohralík (2013)

Equilibrated flux reconstruction when $a = 1$ (linear case)



Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_\ell) \neq f$

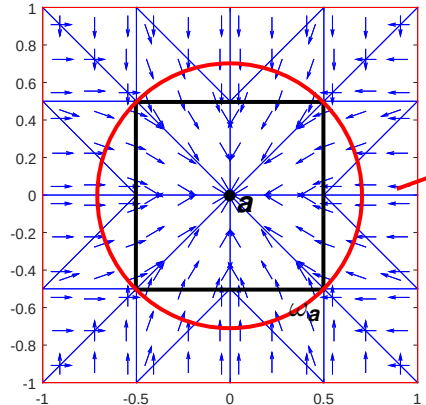
Equilibrated flux reconstruction when $a = 1$ (linear case)

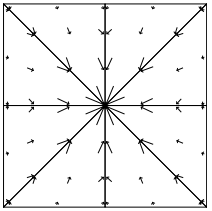


Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$

$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}}$$

Equilibrated flux reconstruction when $a = 1$ (linear case)



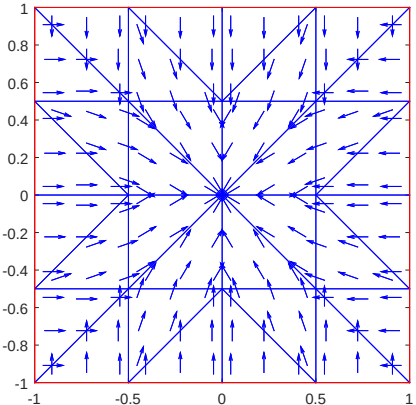


$-\psi_{\boldsymbol{a}} \nabla u_\ell$

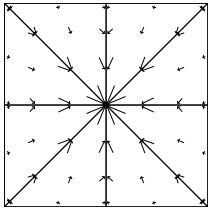
Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla \cdot (-\nabla u_\ell) \neq f$

$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}}$$

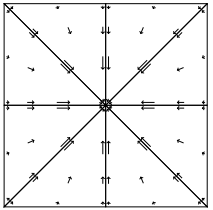
Equilibrated flux reconstruction when $a = 1$ (linear case)



Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$



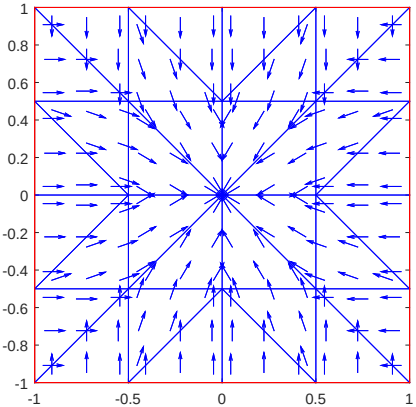
$-\psi_{\boldsymbol{a}} \nabla u_\ell$



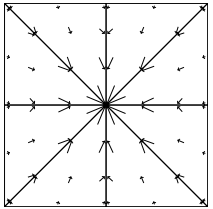
$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}}$

$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}}$$

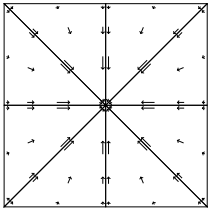
Equilibrated flux reconstruction when $a = 1$ (linear case)



Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$



$-\psi_{\boldsymbol{a}} \nabla u_\ell$

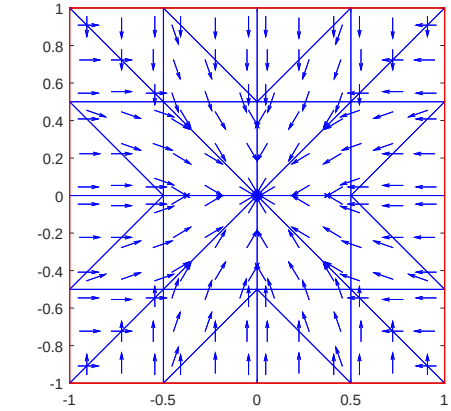


$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}}$

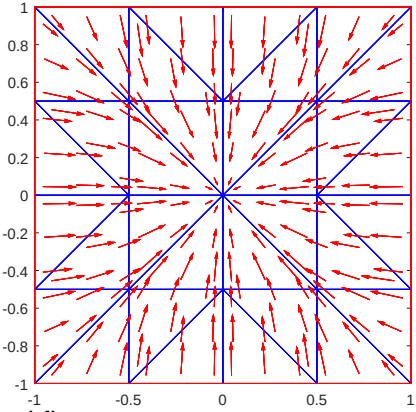
$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}}$$

$$\boldsymbol{\sigma}_\ell^{\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div}, \omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_p(f\psi_{\boldsymbol{a}} - \nabla u_\ell \cdot \nabla \psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}} \nabla u_\ell + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

Equilibrated flux reconstruction when $a = 1$ (linear case)



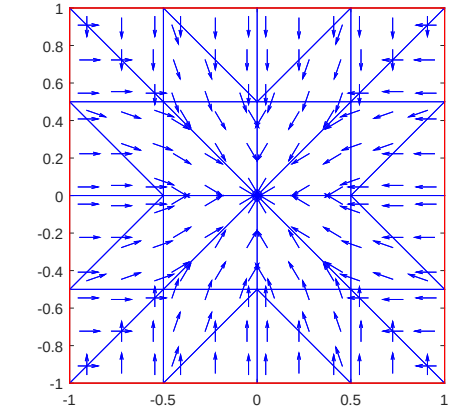
Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$



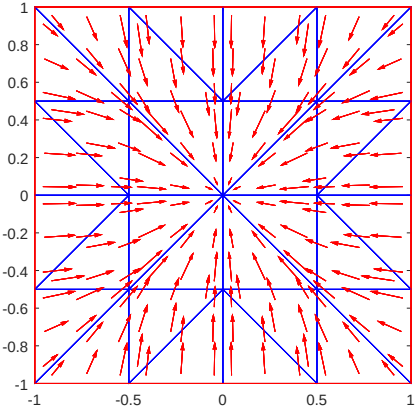
Equilibrated flux rec. $\boldsymbol{\sigma}_\ell$

$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}} \rightarrow \boldsymbol{\sigma}_\ell := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_\ell^{\boldsymbol{a}} \in \mathcal{RT}_p(\mathcal{T}_\ell) \cap \boldsymbol{H}(\mathrm{div}, \Omega), \nabla\cdot\boldsymbol{\sigma}_\ell = \Pi_p f$$

Equilibrated flux reconstruction when $a = 1$ (linear case)



Flux $-\nabla u_\ell \notin \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot(-\nabla u_\ell) \neq f$



Equilibrated flux rec. $\boldsymbol{\sigma}_\ell \in \boldsymbol{H}(\mathrm{div}, \Omega)$, $\nabla\cdot\boldsymbol{\sigma}_\ell = \Pi_p f$

$$\underbrace{-\nabla u_\ell \in \mathcal{RT}_{p-1}(\mathcal{T}_\ell), f \in L^2(\Omega)}_{(f,\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} - (\nabla u_\ell, \nabla\psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = 0 \ \forall \boldsymbol{a} \in \mathcal{V}_\ell^{\mathrm{int}}} \rightarrow \boldsymbol{\sigma}_\ell := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_\ell^{\boldsymbol{a}} \in \mathcal{RT}_p(\mathcal{T}_\ell) \cap \boldsymbol{H}(\mathrm{div}, \Omega), \nabla\cdot\boldsymbol{\sigma}_\ell = \Pi_p f$$

Flux reconstructions (residual liftings)

Definition (**Discretization residual lifting** $\sigma_{\mathrm{disc},\ell}^{k,i}$)

For each $\boldsymbol{a} \in \mathcal{V}_\ell$, solve the local constrained minimization pb

$$\boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i,\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div},\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_p((f - r_\ell^{k,i})\psi_{\boldsymbol{a}} - (\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1})\cdot\nabla\psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}}(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}) + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

and combine

$$\boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i} := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i,\boldsymbol{a}}.$$

Flux reconstructions (residual liftings)

Definition (**Discretization residual lifting** $\sigma_{\mathrm{disc},\ell}^{k,i}$)

For each $\boldsymbol{a} \in \mathcal{V}_\ell$, solve the local constrained minimization pb

$$\boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i,\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div},\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_p((f - r_\ell^{k,i})\psi_{\boldsymbol{a}} - (\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1})\cdot\nabla\psi_{\boldsymbol{a}})}} \|\psi_{\boldsymbol{a}}(\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1}) + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

and combine

$$\boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i} := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_{\mathrm{disc},\ell}^{k,i,\boldsymbol{a}}.$$

Definition (**Linearization residual lifting** $\sigma_{\mathrm{lin},\ell}^{k,i}$)

For each $\boldsymbol{a} \in \mathcal{V}_\ell$, solve the local constrained minimization pb

$$\boldsymbol{\sigma}_{\mathrm{lin},\ell}^{k,i,\boldsymbol{a}} := \arg \min_{\substack{\boldsymbol{v}_\ell \in \mathcal{RT}_p(\mathcal{T}^{\boldsymbol{a}}) \cap \boldsymbol{H}_0(\mathrm{div},\omega_{\boldsymbol{a}}) \\ \nabla\cdot\boldsymbol{v}_\ell = 0}} \|\psi_{\boldsymbol{a}}(a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} - (\boldsymbol{A}_\ell^{k-1}\nabla u_\ell^{k,i} - \boldsymbol{b}_\ell^{k-1})) + \boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}}$$

and combine

$$\boldsymbol{\sigma}_{\mathrm{lin},\ell}^{k,i} := \sum_{\boldsymbol{a}\in\mathcal{V}_\ell} \boldsymbol{\sigma}_{\mathrm{lin},\ell}^{k,i,\boldsymbol{a}}.$$



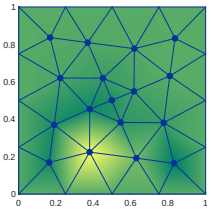
Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^{k,i}_{\mathrm{alg},0} \in \mathcal{P}_1(\mathcal{T}_0) \cap H^1_0(\Omega)$ s.t.

$$(\nabla \rho^{k,i}_{\mathrm{alg},0}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = (r^{k,i}_{\ell}, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} \quad \forall \boldsymbol{a} \in \mathcal{V}_0.$$

- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$



Definition (**Algebraic residual lifting** $\sigma^{k,i}_{\mathrm{alg},\ell}$)

$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} := \arg \min_{\boldsymbol{v}_\ell \in \boldsymbol{V}^{\boldsymbol{a}}_\ell,\, \nabla\cdot\boldsymbol{v}_\ell = \Pi_{Q_\ell}(\psi_{\boldsymbol{a}} r^{k,i}_{\ell} - \nabla\psi_{\boldsymbol{a}}\cdot\nabla\rho^{k,i}_{\mathrm{alg},0})} \|\boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}},$$

- lifting the algebraic residual $r^{k,i}_{\ell}$

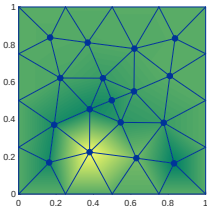
Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^{k,i}_{\mathrm{alg},0} \in \mathcal{P}_1(\mathcal{T}_0) \cap H^1_0(\Omega)$ s.t.

$$(\nabla \rho^{k,i}_{\mathrm{alg},0}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = (r^{k,i}_{\ell}, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} \quad \forall \boldsymbol{a} \in \mathcal{V}_0.$$

- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$



Definition (**Algebraic residual lifting** $\sigma^{k,i}_{\mathrm{alg},\ell}$)

$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} := \arg \min_{\boldsymbol{v}_\ell \in \boldsymbol{V}^{\boldsymbol{a}}_\ell,\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_{Q_\ell}(\psi_{\boldsymbol{a}} r^{k,i}_{\ell} - \nabla\psi_{\boldsymbol{a}}\cdot\nabla\rho^{k,i}_{\mathrm{alg},0})} \|\boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}},$$

$$\sigma^{k,i}_{\mathrm{alg},\ell} := \sum_{\boldsymbol{a}\in\mathcal{V}_0} \sigma^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell}$$

- lifting the algebraic residual $r^{k,i}_{\ell}$
- $\nabla\cdot\sigma^{k,i}_{\mathrm{alg},\ell} = \sum_{\boldsymbol{a}\in\mathcal{V}_0} \nabla\cdot\sigma^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} = \Pi_{Q_\ell} r^{k,i}_{\ell} = r^{k,i}_{\ell}$

Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^{k,i}_{\mathrm{alg},0} \in \mathcal{P}_1(\mathcal{T}_0) \cap H^1_0(\Omega)$ s.t.

$$(\nabla \rho^{k,i}_{\mathrm{alg},0}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = (r^{k,i}_\ell, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} \quad \forall \boldsymbol{a} \in \mathcal{V}_0.$$

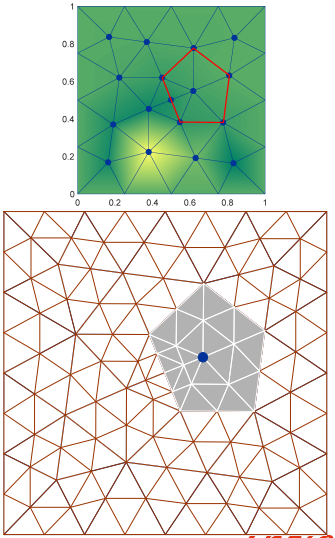
- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$

Definition (**Algebraic residual lifting** $\sigma^{k,i}_{\mathrm{alg},\ell}$)

$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} := \arg \min_{\boldsymbol{v}_\ell \in \boldsymbol{V}^{\boldsymbol{a}}_\ell,\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_{Q_\ell}(\psi_{\boldsymbol{a}} r^{k,i}_\ell - \nabla\psi_{\boldsymbol{a}}\cdot\nabla\rho^{k,i}_{\mathrm{alg},0})} \|\boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}},$$

$$\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} := \sum_{\boldsymbol{a}\in\mathcal{V}_0} \boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell}$$

- lifting the algebraic residual $r^{k,i}_\ell$
- $\nabla\cdot\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} = \sum_{\boldsymbol{a}\in\mathcal{V}_0} \nabla\cdot\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} = \Pi_{Q_\ell} r^{k,i}_\ell = r^{k,i}_\ell$



Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^{k,i}_{\mathrm{alg},0} \in \mathcal{P}_1(\mathcal{T}_0) \cap H^1_0(\Omega)$ s.t.

$$(\nabla \rho^{k,i}_{\mathrm{alg},0}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = (r^{k,i}_{\ell}, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} \quad \forall \boldsymbol{a} \in \mathcal{V}_0.$$

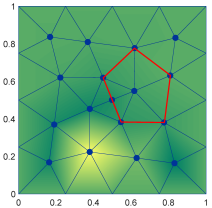
- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$

Definition (Algebraic residual lifting $\sigma^{k,i}_{\mathrm{alg},\ell}$)

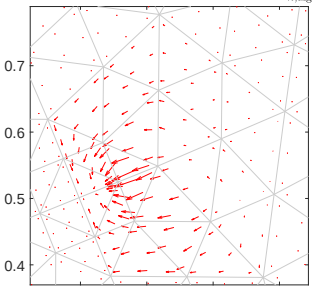
$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} := \arg \min_{\boldsymbol{v}_\ell \in \boldsymbol{V}^{\boldsymbol{a}}_\ell,\ \nabla\cdot\boldsymbol{v}_\ell = \Pi_{Q_\ell}(\psi_{\boldsymbol{a}} r^{k,i}_\ell - \nabla\psi_{\boldsymbol{a}}\cdot\nabla\rho^{k,i}_{\mathrm{alg},0})} \|\boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}},$$

$$\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} := \sum_{\boldsymbol{a}\in\mathcal{V}_0} \boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell}$$

- lifting the algebraic residual $r^{k,i}_\ell$
- $\nabla\cdot\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} = \sum_{\boldsymbol{a}\in\mathcal{V}_0} \nabla\cdot\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} = \Pi_{Q_\ell} r^{k,i}_\ell = r^{k,i}_\ell$



local alg. error flux reconstruction, $\sigma^{\mathrm{a},i}_{h,\mathrm{alg}}$



Algebraic error flux reconstruction, two-level setting

Definition (Coarse grid solve)

Find $\rho^{k,i}_{\mathrm{alg},0} \in \mathcal{P}_1(\mathcal{T}_0) \cap H^1_0(\Omega)$ s.t.

$$(\nabla \rho^{k,i}_{\mathrm{alg},0}, \nabla \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} = (r^{k,i}_{\ell}, \psi_{\boldsymbol{a}})_{\omega_{\boldsymbol{a}}} \quad \forall \boldsymbol{a} \in \mathcal{V}_0.$$

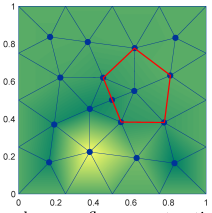
- $\mathcal{P}_1$ FE solve on coarse mesh $\mathcal{T}_0$

Definition (**Algebraic residual lifting** $\sigma^{k,i}_{\mathrm{alg},\ell}$)

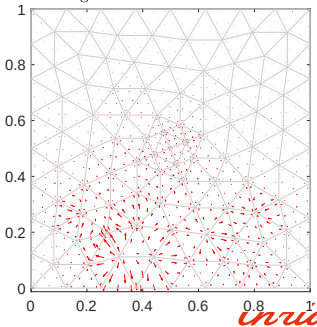
$$\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} := \arg \min_{\boldsymbol{v}_\ell \in \boldsymbol{V}^{\boldsymbol{a}}_{\ell}, \nabla\cdot\boldsymbol{v}_\ell = \Pi_{Q_\ell}(\psi_{\boldsymbol{a}} r^{k,i}_{\ell} - \nabla\psi_{\boldsymbol{a}}\cdot\nabla\rho^{k,i}_{\mathrm{alg},0})} \|\boldsymbol{v}_\ell\|_{\omega_{\boldsymbol{a}}},$$

$$\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} := \sum_{\boldsymbol{a}\in\mathcal{V}_0} \boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell}$$

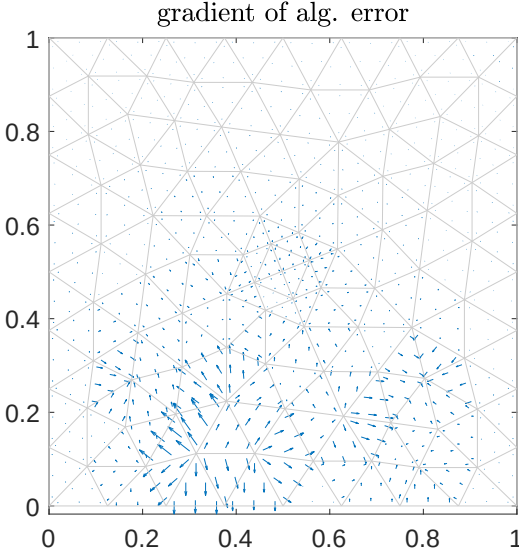
- lifting the algebraic residual $r^{k,i}_{\ell}$
- $\nabla\cdot\boldsymbol{\sigma}^{k,i}_{\mathrm{alg},\ell} = \sum_{\boldsymbol{a}\in\mathcal{V}_0} \nabla\cdot\boldsymbol{\sigma}^{k,i,\boldsymbol{a}}_{\mathrm{alg},\ell} = \Pi_{Q_\ell} r^{k,i}_{\ell} = r^{k,i}_{\ell}$

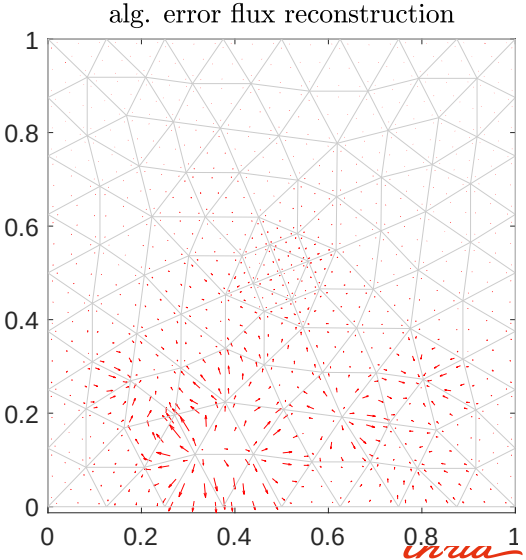


alg. error flux reconstruction



Algebraic error flux reconstruction, two-level setting





A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate, A. Ern, M. Vohralík (2013))

Let $u_\ell^{k,i} \in V_\ell^p$ be given.



A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate, A. Ern, M. Vohralík (2013))

Let $u_\ell^{k,i} \in V_\ell^p$ *be given. Let*

$$\underbrace{\boldsymbol{\sigma}_\ell^{k,i}}_{\text{total}} := \underbrace{\boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}}_{\text{discretization}} + \underbrace{\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}}_{\text{linearization}} + \underbrace{\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}}_{\text{algebraic}} .$$



A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate, A. Ern, M. Vohralík (2013))

Let $u_\ell^{k,i} \in V_\ell^p$ *be given. Let* $\underbrace{\boldsymbol{\sigma}_\ell^{k,i}}_{\text{total}} := \underbrace{\boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}}_{\text{discretization}} + \underbrace{\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}}_{\text{linearization}} + \underbrace{\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}}_{\text{algebraic}}$. *Then* $\boldsymbol{\sigma}_\ell^{k,i} \in \boldsymbol{H}(\mathrm{div}, \Omega)$ *is such that* $\nabla \cdot \boldsymbol{\sigma}_\ell^{k,i} = f$



A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate, A. Ern, M. Vohralík (2013))

Let $u_\ell^{k,i} \in V_\ell^p$ *be given. Let* $\underbrace{\boldsymbol{\sigma}_\ell^{k,i}}_{\text{total}} := \underbrace{\boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}}_{\text{discretization}} + \underbrace{\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}}_{\text{linearization}} + \underbrace{\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}}_{\text{algebraic}}$. *Then* $\boldsymbol{\sigma}_\ell^{k,i} \in$ $\boldsymbol{H}(\mathrm{div},\Omega)$ *is such that* $\nabla\cdot\boldsymbol{\sigma}_\ell^{k,i} = f$ *and there holds the* ***guaranteed upper bound***

$$
\begin{aligned}
|||u - u_\ell^{k,i}||| &\le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_\ell^{k,i}\|}_{\eta\left(u_\ell^{k,i}\right)} \\
&\le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}\|}_{\eta_{\text{disc}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}\|}_{\eta_{\text{lin}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}\|}_{\eta_{\text{alg}}\left(u_\ell^{k,i}\right)}.
\end{aligned}
$$



A posteriori error estimate distinguishing the error components

Theorem (A posteriori error estimate, A. Ern, M. Vohralík (2013))

Let $u_\ell^{k,i} \in V_\ell^p$ *be given. Let* $\underbrace{\boldsymbol{\sigma}_\ell^{k,i}}_{\text{total}} := \underbrace{\boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}}_{\text{discretization}} + \underbrace{\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}}_{\text{linearization}} + \underbrace{\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}}_{\text{algebraic}}$. *Then* $\boldsymbol{\sigma}_\ell^{k,i} \in \boldsymbol{H}(\mathrm{div},\Omega)$ *is such that* $\nabla\cdot\boldsymbol{\sigma}_\ell^{k,i} = f$ *and there holds the* ***guaranteed upper bound***

$$|||u - u_\ell^{k,i}||| \le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_\ell^{k,i}\|}_{\eta\left(u_\ell^{k,i}\right)}$$

$$\le \underbrace{\|a(|\nabla u_\ell^{k,i}|)\nabla u_\ell^{k,i} + \boldsymbol{\sigma}_{\text{disc},\ell}^{k,i}\|}_{\eta_{\text{disc}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{lin},\ell}^{k,i}\|}_{\eta_{\text{lin}}\left(u_\ell^{k,i}\right)} + \underbrace{\|\boldsymbol{\sigma}_{\text{alg},\ell}^{k,i}\|}_{\eta_{\text{alg}}\left(u_\ell^{k,i}\right)}.$$

Moreover, the estimates are ***locally efficient*** *and* ***robust*** *with respect to the* ***strength of nonlinearities***

$$\eta_K\left(u_\ell^{k,i}\right) \le C_{\text{eff}}|||u - u_\ell^{k,i}|||_{\omega_K} \qquad \forall K \in \mathcal{T}_\ell, \qquad C_{\text{eff}} \text{ independent of } \frac{a_{\text{c}}}{a_{\text{m}}}.$$



Outline

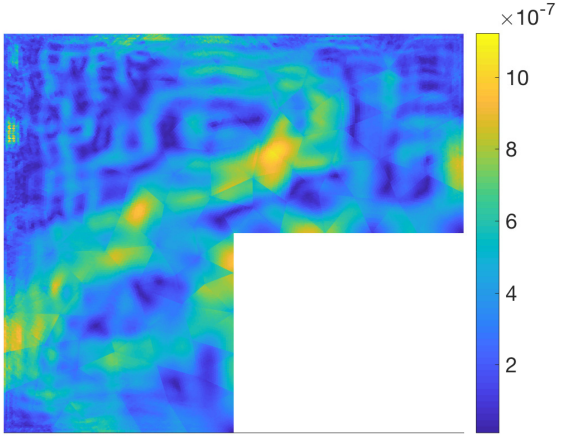
1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

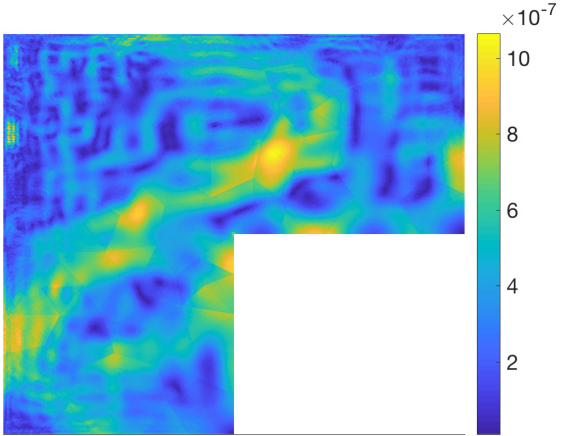
3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions

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



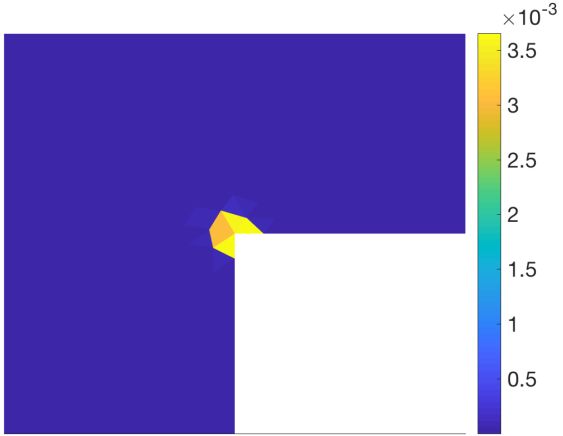
Estimated algebraic errors $\eta_{\mathrm{alg},K}(u_\ell^i)$



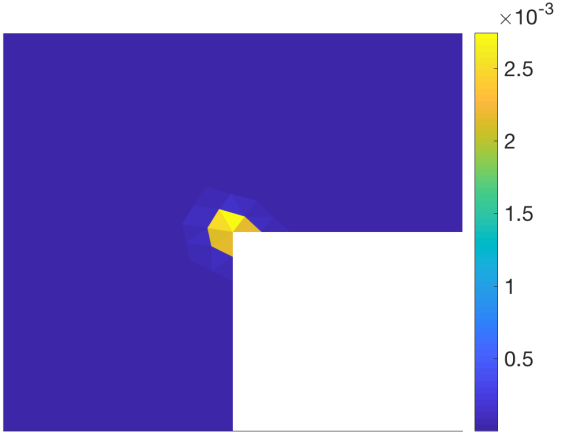
Exact algebraic errors $\|\nabla(u_\ell - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

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



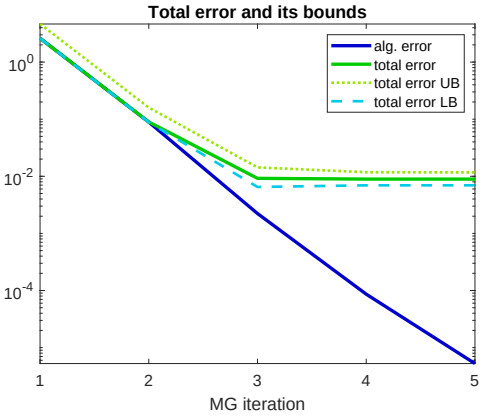
Estimated total errors $\eta_K(u_\ell^i)$



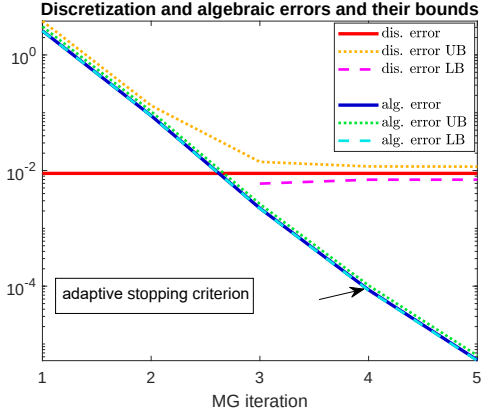
Exact total errors $\|\nabla(u - u_\ell^i)\|_K$

J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Including **algebraic error**: $\mathbb{A}_\ell \mathrm{U}_\ell^i \neq \mathrm{F}_\ell$



Total error



Error components and adaptive st. crit.

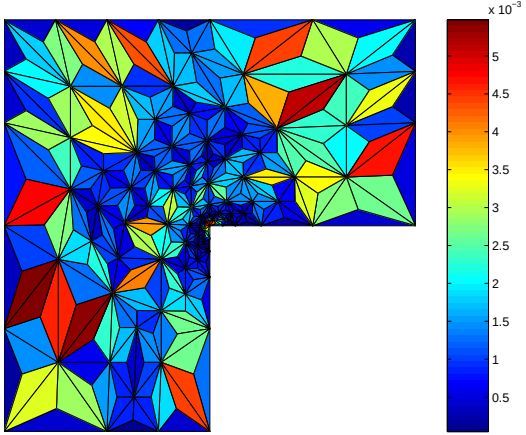
J. Papež, U. Rüde, M. Vohralík, B. Wohlmuth, Computer Methods in Applied Mechanics and Engineering (2020)

Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including linearization and algebraic error: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,l}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,l} \neq \mathrm{F}_\ell^{k-1}$

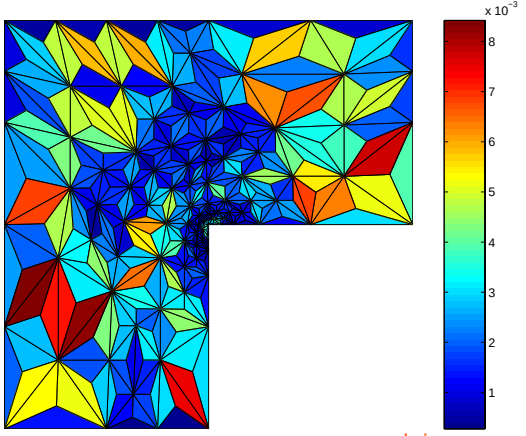
Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including **linearization** and **algebraic error**: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$

Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including **linearization** and **algebraic error**: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$

Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including **linearization** and **algebraic error**: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$



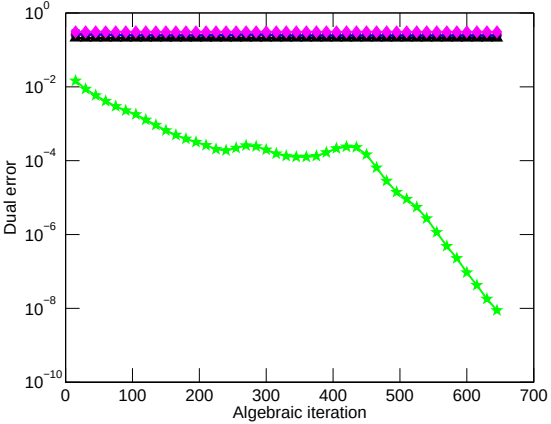
Estimated errors $\eta_K(u_\ell^{k,i})$



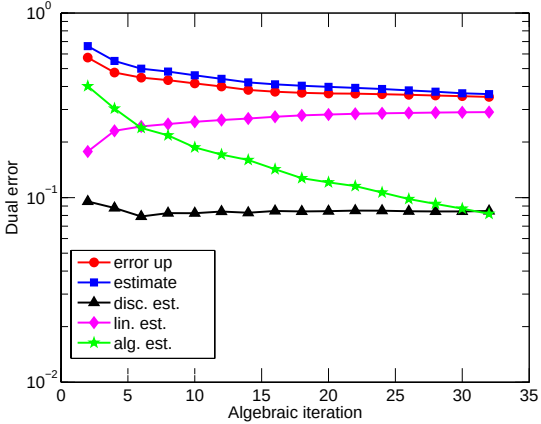
Exact errors $\|\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_\ell^{k,i})\|_{q,K}$

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

Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including **linearization** and **algebraic error**: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$



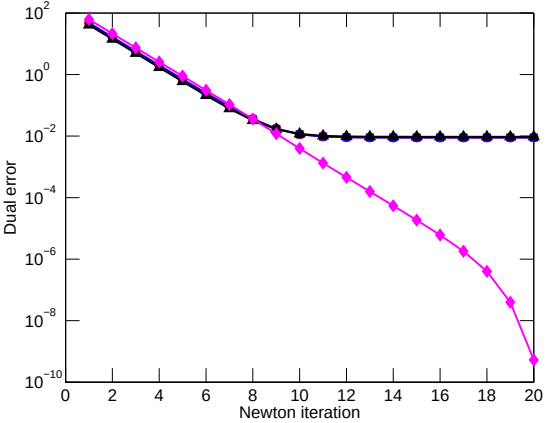
Newton



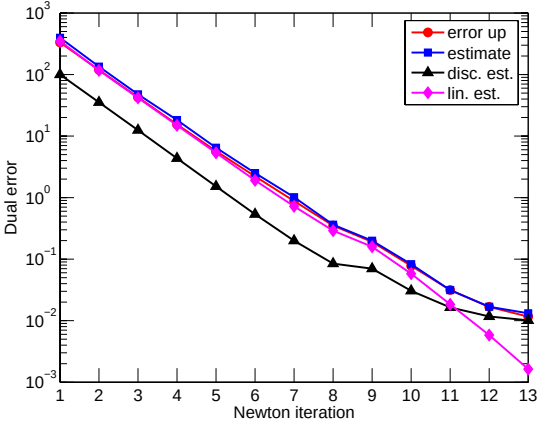
adaptive inexact Newton

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

Nonlinear pb $-\nabla\cdot(a|\nabla u|)(\nabla u) = f$: including **linearization** and **algebraic error**: $\mathcal{A}_\ell(\mathrm{U}_\ell^{k,i}) \neq \mathrm{F}_\ell$, $\mathbb{A}_\ell^{k-1}\mathrm{U}_\ell^{k,i} \neq \mathrm{F}_\ell^{k-1}$



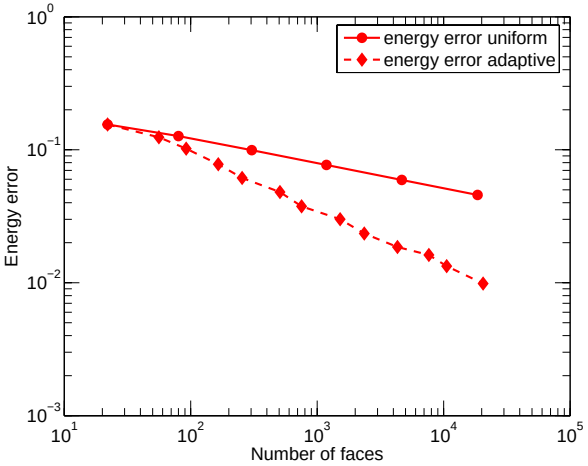
Newton



adaptive inexact Newton

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

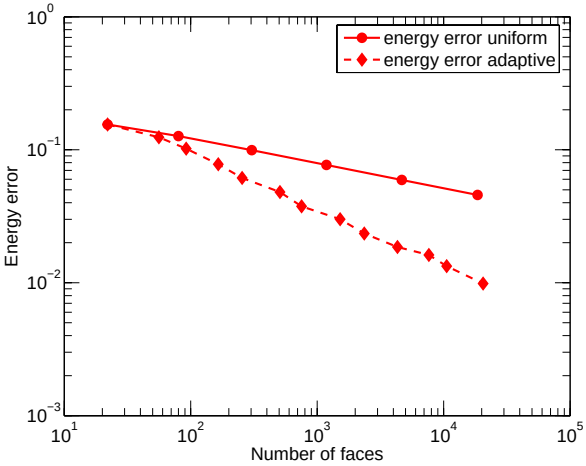
Optimal decay rate wrt degrees of freedom & computational cost



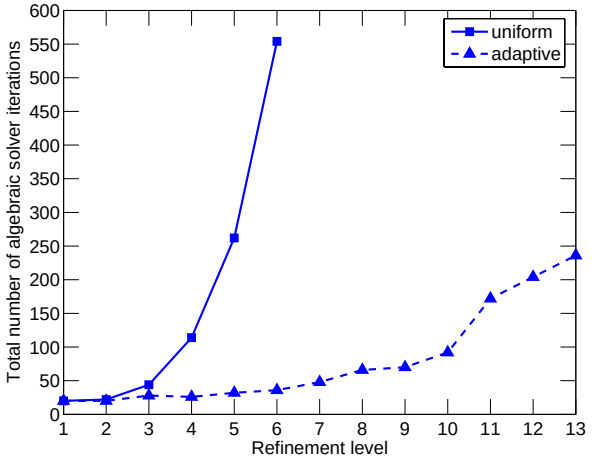
Optimal decay rate wrt DoFs

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

Optimal decay rate wrt degrees of freedom & computational cost



Optimal decay rate wrt DoFs



Optimal computational cost

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

Adaptivity of error components: optimality in numerical simulations

Theorem (Optimal numerical simulation, A. Haberl, D. Praetorius, S. Schimanko, M. Vohralík (2021)**)**

***Best-possible decay rate** of the **error** with respect to the **cost** is achieved:*

$$|||u - u_{\ell}^{\bar{k},\bar{i}}||| \lesssim \left\{ \sum_{\ell=0}^{\bar{\ell}} \sum_{k=0}^{\bar{k}} \sum_{i=0}^{\bar{i}} |V_{\ell}^{p}| \right\}^{-p/d}$$

(replaces traditional h^p, even for singular u).

Outline

1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions



Two-phase flow

Incompressible two-phase flow in porous media

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

$$\partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\boldsymbol{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) = q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\},$$
$$s_\mathrm{g} + s_\mathrm{w} = 1,$$
$$p_\mathrm{g} - p_\mathrm{w} = p_\mathrm{c}(s_\mathrm{w})$$

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

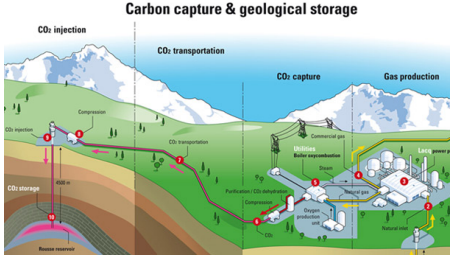
Two-phase flow

Incompressible two-phase flow in porous media

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

$$\partial_t(\phi s_\alpha) - \nabla\cdot\left(\frac{k_{\mathrm{r},\alpha}(s_\mathrm{w})}{\mu_\alpha}\boldsymbol{K}(\nabla p_\alpha + \rho_\alpha g \nabla z)\right) = q_\alpha, \qquad \alpha \in \{\mathrm{g}, \mathrm{w}\},$$
$$s_\mathrm{g} + s_\mathrm{w} = 1,$$
$$p_\mathrm{g} - p_\mathrm{w} = p_\mathrm{c}(s_\mathrm{w})$$

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



Outline

1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions

Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance, I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík (2020))

There holds

$$\text{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta_{\mathrm{sp},c}^{n,j,k,i} + \eta_{\mathrm{tm},c}^{n,j,k,i} + \eta_{\mathrm{reg},c}^{n,j,k,i} + \eta_{\mathrm{lin},c}^{n,j,k,i} + \eta_{\mathrm{alg},c}^{n,j,k,i} \right)^2 \right\}^{1/2}.$$

Error components

- $\eta_{\mathrm{sp},c}^{n,j,k,i}$: spatial discretization
- $\eta_{\mathrm{tm},c}^{n,j,k,i}$: temporal discretization
- $\eta_{\mathrm{reg},c}^{n,j,k,i}$: regularization
- $\eta_{\mathrm{lin},c}^{n,j,k,i}$: linearization
- $\eta_{\mathrm{alg},c}^{n,j,k,i}$: algebraic solver

Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering**

Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance, I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík (2020))

There holds

$$\text{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta_{\mathrm{sp},c}^{n,j,k,i} + \eta_{\mathrm{tm},c}^{n,j,k,i} + \eta_{\mathrm{reg},c}^{n,j,k,i} + \eta_{\mathrm{lin},c}^{n,j,k,i} + \eta_{\mathrm{alg},c}^{n,j,k,i} \right)^2 \right\}^{1/2}.$$

Error components

- $\eta_{\mathrm{sp},c}^{n,j,k,i}$: spatial discretization
- $\eta_{\mathrm{tm},c}^{n,j,k,i}$: temporal discretization
- $\eta_{\mathrm{reg},c}^{n,j,k,i}$: regularization
- $\eta_{\mathrm{lin},c}^{n,j,k,i}$: linearization
- $\eta_{\mathrm{alg},c}^{n,j,k,i}$: algebraic solver

Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering**

Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance, I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík (2020)**)**

There holds

$$\text{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta_{\mathrm{sp},c}^{n,j,k,i} + \eta_{\mathrm{tm},c}^{n,j,k,i} + \eta_{\mathrm{reg},c}^{n,j,k,i} + \eta_{\mathrm{lin},c}^{n,j,k,i} + \eta_{\mathrm{alg},c}^{n,j,k,i} \right)^2 \right\}^{1/2}.$$

Error components

- $\eta_{\mathrm{sp},c}^{n,j,k,i}$: spatial discretization
- $\eta_{\mathrm{tm},c}^{n,j,k,i}$: temporal discretization
- $\eta_{\mathrm{reg},c}^{n,j,k,i}$: regularization
- $\eta_{\mathrm{lin},c}^{n,j,k,i}$: linearization
- $\eta_{\mathrm{alg},c}^{n,j,k,i}$: algebraic solver

Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering**

Multi-phase multi-compositional flow

Theorem (Multi-phase multi-compositional Darcy flow with phase (dis)appearance, I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík (2020)**)**

There holds

$$\text{error on time interval } I_n \leq \left\{ \sum_{c \in \mathcal{C}} \left(\eta_{\mathrm{sp},c}^{n,j,k,i} + \eta_{\mathrm{tm},c}^{n,j,k,i} + \eta_{\mathrm{reg},c}^{n,j,k,i} + \eta_{\mathrm{lin},c}^{n,j,k,i} + \eta_{\mathrm{alg},c}^{n,j,k,i} \right)^2 \right\}^{1/2}.$$

Error components

- $\eta_{\mathrm{sp},c}^{n,j,k,i}$: spatial discretization
- $\eta_{\mathrm{tm},c}^{n,j,k,i}$: temporal discretization
- $\eta_{\mathrm{reg},c}^{n,j,k,i}$: regularization
- $\eta_{\mathrm{lin},c}^{n,j,k,i}$: linearization
- $\eta_{\mathrm{alg},c}^{n,j,k,i}$: algebraic solver

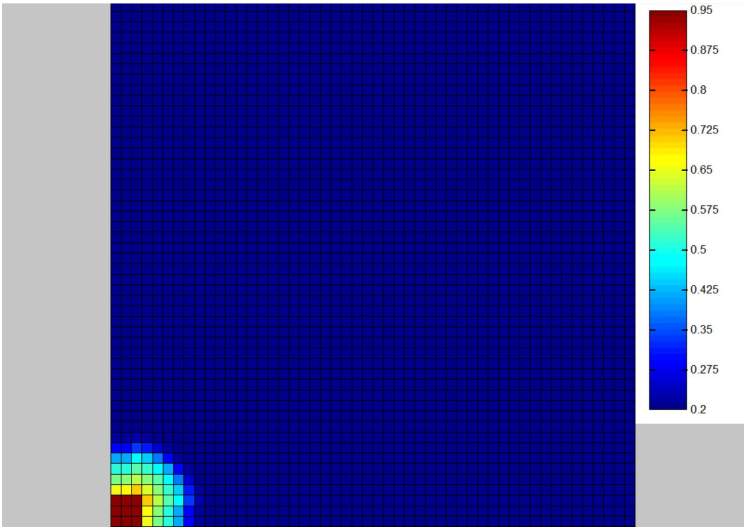
Error control

- at **any moment** during the simulation
- price: sparse **matrix-vector** multiplication

Full adaptivity

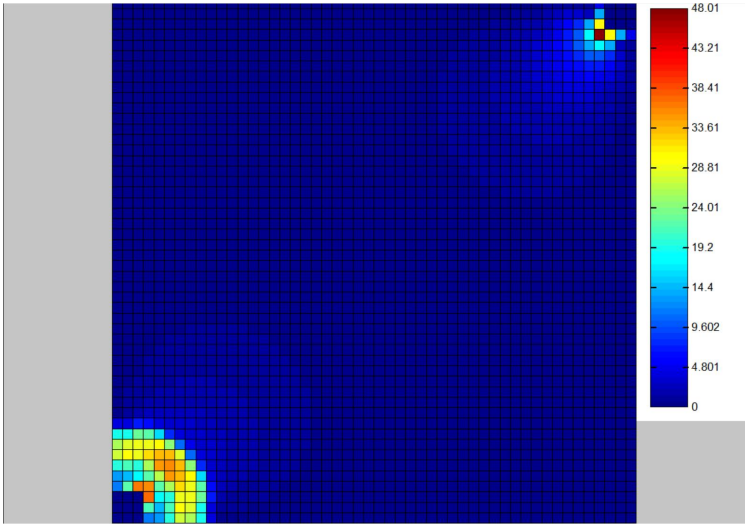
- **same physical units** of all component estimators
- **balance** all component estimators
- **online steering**

Academic example of oil recovery



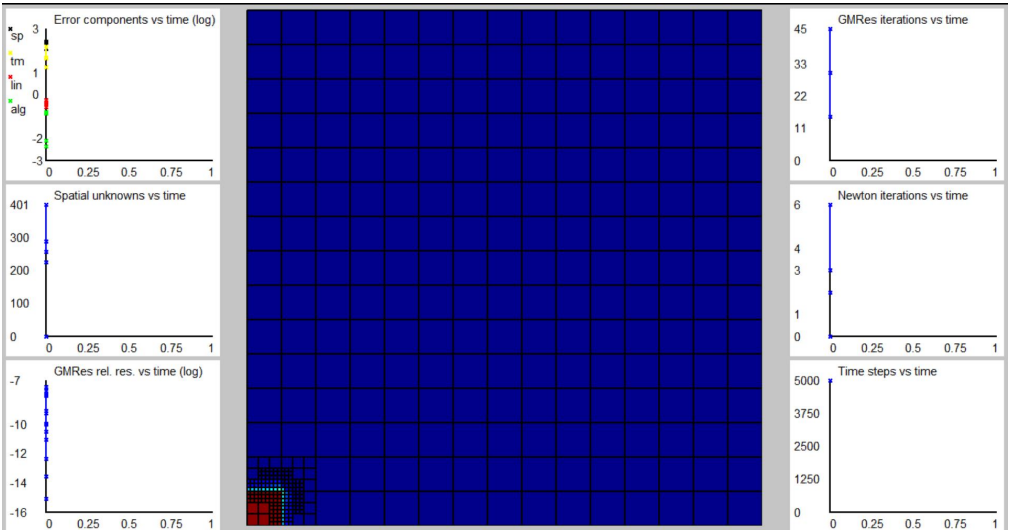
M. Vohralík, M. F. Wheeler, Computational Geosciences (2013)

Academic example of oil recovery, **overall a posteriori estimate**



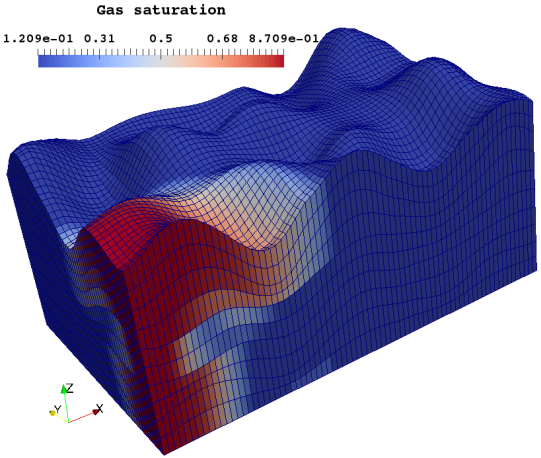
M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Academic example of oil recovery, **adaptivity of error components**

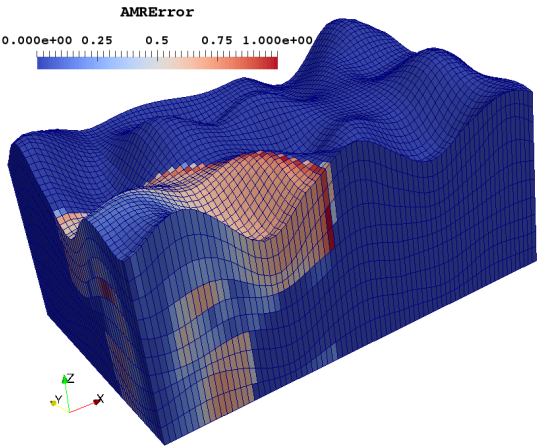


M. Vohralík, M. Wheeler, Computational Geosciences (2013)

Real-world example: 3 phases, 3 components (black-oil) problem



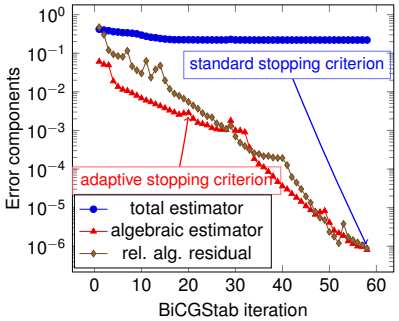
Gas saturation

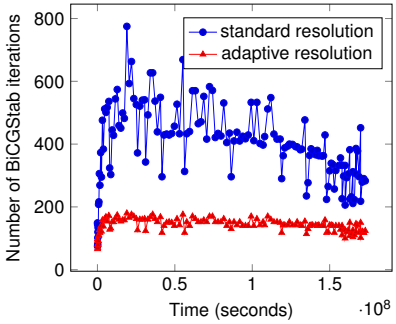


A posteriori error estimate

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Three-phases, three-components (black-oil) problem: algebraic solver & spatial mesh adaptivity

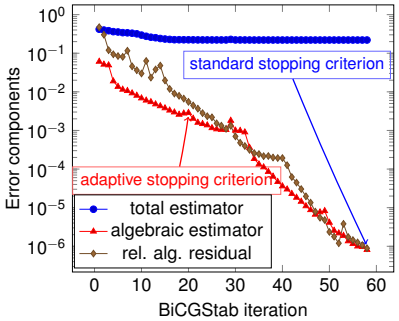


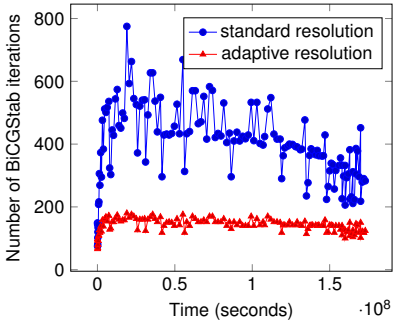


	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Three-phases, three-components (black-oil) problem: algebraic solver & spatial mesh adaptivity

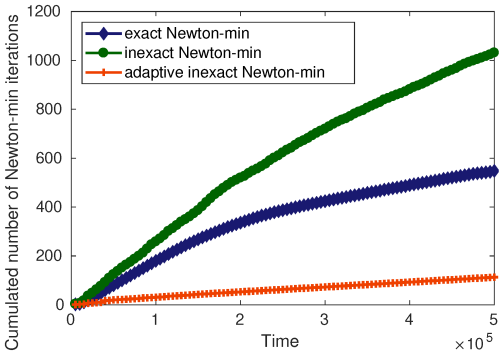


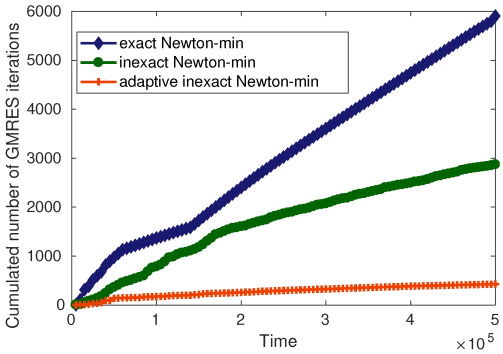


	Linear solver steps	Resolution time	AMR time	Estimators evaluation	Gain factor
Standard resolution	66386	1023s	-	-	-
Adaptive resolution	20184	201s	42s	26s	3.8

M. Vohralík, S. Yousef, Computer Methods in Applied Mechanics and Engineering (2018)

Phase (dis)appearance: Couplex-gas benchmark

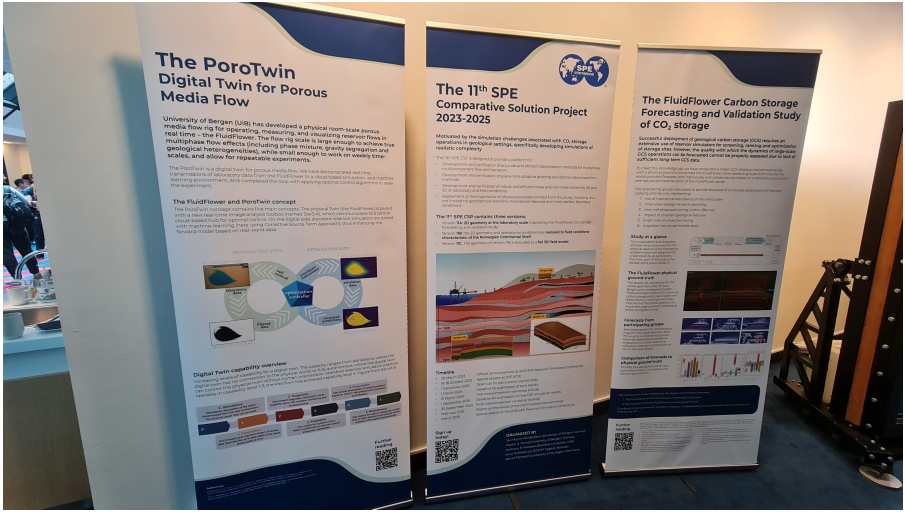




Adaptive linear and nonlinear solvers

I. Ben Gharbia, J. Dabaghi, V. Martin, M. Vohralík, Computational Geosciences (2020)

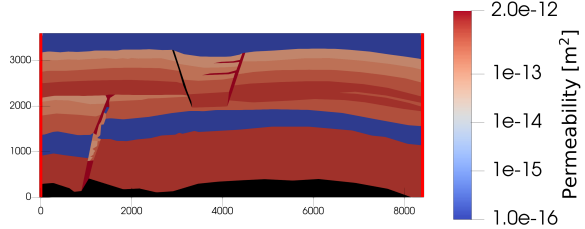
SIAM Conference on Mathematical & Computational Issues in the Geosciences, Bergen, June 2023: the FluidFlower experiment



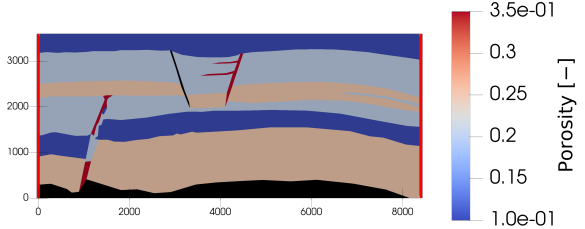
SIAM Conference on Mathematical & Computational Issues in the Geosciences, Bergen, June 2023: the FluidFlower experiment



Geological sequestration of CO_2

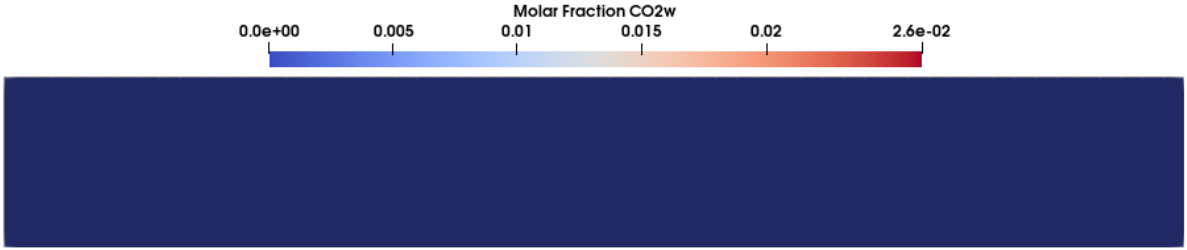


FluidFlower permeability



FluidFlower porosity

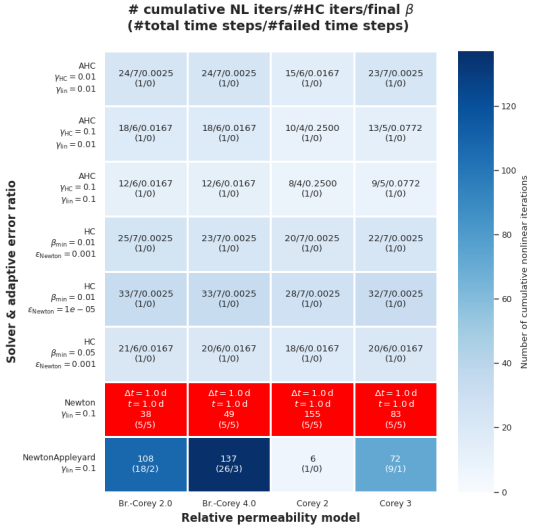
Geological sequestration of CO_2



CO_2 molar fraction

E. Flauraud, I. Lannabi, M. Vohralík, S. Yousef, in preparation (2026)

Geological sequestration of CO_2: adaptivity of error components



P. von Schultzendorff, J. W. Both, J. M. Nordbotten, T. H. Sandve, M. Vohralík, submitted (2026)

Outline

1 Introduction
- Textbook numerical approximation and analysis
- Adaptive numerical approximation and analysis
- Motivations
- Crucial questions and answers
- Achievements and example results

2 Steady nonlinear diffusion
- A posteriori error estimates (overall and components)
- Adaptivity of error components: mesh and solvers

3 Multiphase multicompositional flows
- Error control and adaptivity of error components

4 Conclusions

Conclusions

- **adaptivity** : space/time mesh,

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **error control**

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**
- **optimal** (best-possible) **decay rate** of the error wrt the computational **cost**

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**
- **optimal** (best-possible) **decay rate** of the error wrt the computational **cost**
- not a novel scheme, rather an **efficient use** of existing **building blocks**

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**
- **optimal** (best-possible) **decay rate** of the error wrt the computational **cost**
- not a novel scheme, rather an **efficient use** of existing **building blocks**
- recovering **mass balance** in any situation

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**
- **optimal** (best-possible) **decay rate** of the error wrt the computational **cost**
- not a novel scheme, rather an **efficient use** of existing **building blocks**
- recovering **mass balance** in any situation

BEN GHARBIA I., DABAGHI J., MARTIN V., VOHRALÍK M., A posteriori error estimates for a compositional two-phase flow with nonlinear complementarity constraints, *Comput. Geosci.* **24** (2020), 1031–1055.

ERN A., VOHRALÍK M., Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations, *SIAM J. Numer. Anal.* **53** (2015), 1058–1081.

ERN A., VOHRALÍK M., Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs, *SIAM J. Sci. Comput.* **35** (2013), A1761–A1791.

HABERL A., PRAETORIUS D., SCHIMANKO S., VOHRALÍK M., Convergence and quasi-optimal cost of adaptive algorithms for nonlinear operators including iterative linearization and algebraic solver, *Numer. Math.* **147** (2021), 679–725.

MITRA K., VOHRALÍK M. Guaranteed, locally efficient, and robust a posteriori estimates for nonlinear elliptic problems in iteration-dependent norms. An orthogonal decomposition result based on iterative linearization. *Numer. Math.*, DOI 10.1007/s00211-026-01578-8, 2026.

PAPEŽ J., RÜDE U., VOHRALÍK M., WOHLMUTH B., Sharp algebraic and total a posteriori error bounds for h and p finite elements via a multilevel approach. Recovering mass balance in any situation, *Comput. Methods Appl. Mech. Engrg.* **371** (2020), 113243.

VOHRALÍK M., WHEELER M. F., A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows, *Comput. Geosci.* **17** (2013), 789–812.

Conclusions

- **adaptivity of error components**: space/time mesh, (non)linear solver, regularization
- a posteriori **overall error control**
- **optimal** (best-possible) **decay rate** of the error wrt the computational **cost**
- not a novel scheme, rather an **efficient use** of existing **building blocks**
- recovering **mass balance** in any situation

BEN GHARBIA I., DABAGHI J., MARTIN V., VOHRALÍK M., A posteriori error estimates for a compositional two-phase flow with nonlinear complementarity constraints, *Comput. Geosci.* **24** (2020), 1031–1055.

ERN A., VOHRALÍK M., Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations, *SIAM J. Numer. Anal.* **53** (2015), 1058–1081.

ERN A., VOHRALÍK M., Adaptive inexact Newton methods with a posteriori stopping criteria for nonlinear diffusion PDEs, *SIAM J. Sci. Comput.* **35** (2013), A1761–A1791.

HABERL A., PRAETORIUS D., SCHIMANKO S., VOHRALÍK M., Convergence and quasi-optimal cost of adaptive algorithms for nonlinear operators including iterative linearization and algebraic solver, *Numer. Math.* **147** (2021), 679–725.

MITRA K., VOHRALÍK M. Guaranteed, locally efficient, and robust a posteriori estimates for nonlinear elliptic problems in iteration-dependent norms. An orthogonal decomposition result based on iterative linearization. *Numer. Math.*, DOI 10.1007/s00211-026-01578-8, 2026.

PAPEŽ J., RÜDE U., VOHRALÍK M., WOHLMUTH B., Sharp algebraic and total a posteriori error bounds for h and p finite elements via a multilevel approach. Recovering mass balance in any situation, *Comput. Methods Appl. Mech. Engrg.* **371** (2020), 113243.

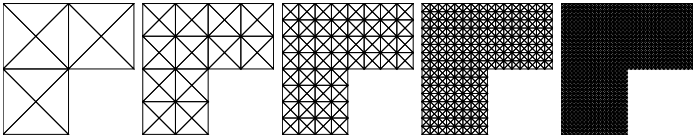
VOHRALÍK M., WHEELER M. F., A posteriori error estimates, stopping criteria, and adaptivity for two-phase flows, *Comput. Geosci.* **17** (2013), 789–812.

Thank you for your attention!

Outline

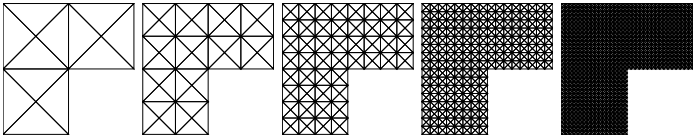
- Model nonlinearities
- Nonsmooth and degenerate nonlinearities

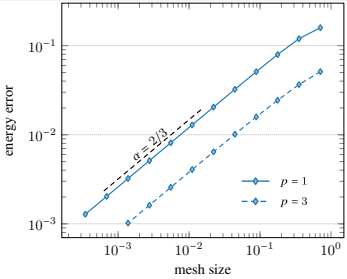
Adaptivity of error components: optimality in numerical simulations



(courtesy D. Praetorius, TU Wien)

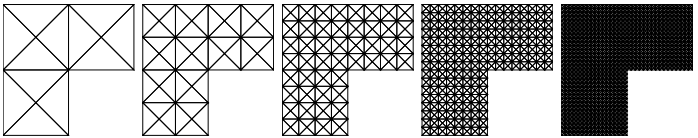
Adaptivity of error components: optimality in numerical simulations

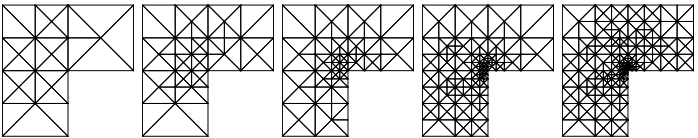


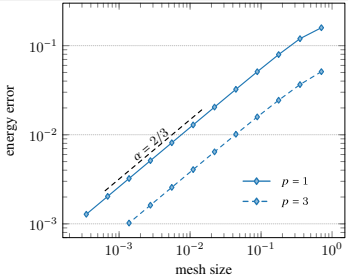


(courtesy D. Praetorius, TU Wien)

Adaptivity of error components: optimality in numerical simulations

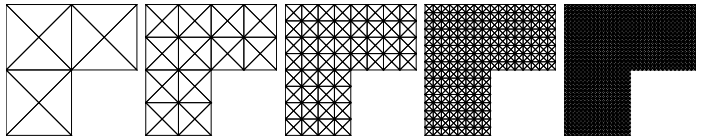


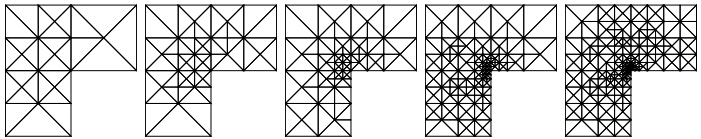




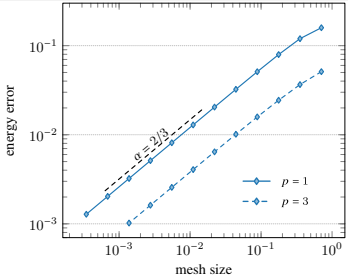
(courtesy D. Praetorius, TU Wien)

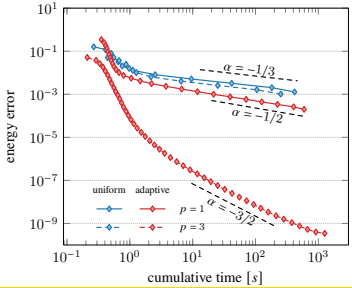
Adaptivity of error components: optimality in numerical simulations





(courtesy D. Praetorius, TU Wien)



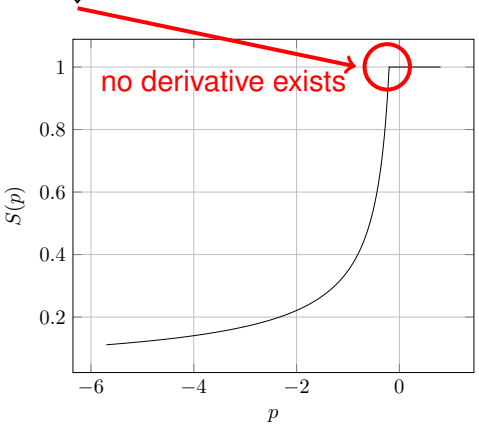


Outline

- Model nonlinearities
- Nonsmooth and degenerate nonlinearities

Nonsmooth and degenerate nonlinearities

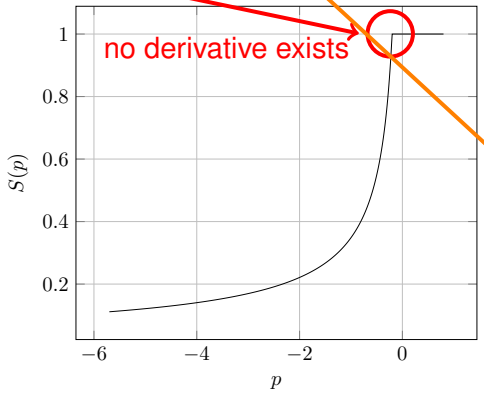
Nonsmooth **nonlinearities**



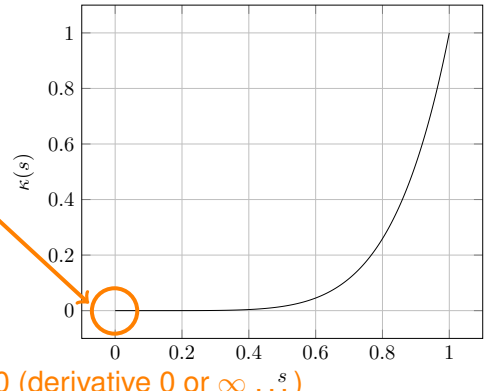
Brooks–Corey pressure–saturation function

Nonsmooth and degenerate nonlinearities

Nonsmooth and degenerate nonlinearities



Brooks–Corey pressure–saturation function



value 0 (derivative 0 or ∞ ...)

Brooks–Corey saturation–relative permeability function

Nonsmooth and degenerate nonlinearities

Nonsmooth and degenerate nonlinearities

- omnipresent in applications
- cause **convergence troubles** of **standard iterative linearization methods**

Nonsmooth and degenerate nonlinearities: common recipes

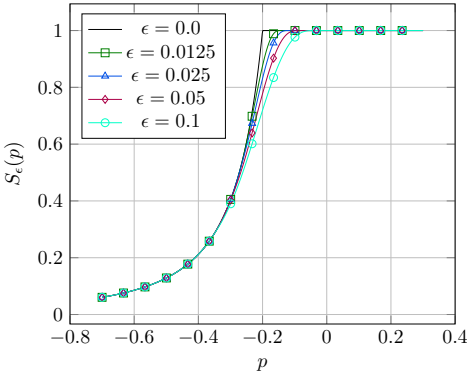
Nonsmooth and degenerate nonlinearities

- omnipresent in applications
- cause **convergence troubles** of **standard iterative linearization methods**

Common recipes

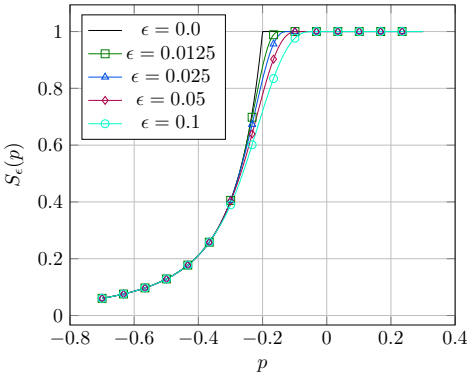
- timestep cutting
- damping
- scheme switching (from Newton to fixed-point . . .)
- variable switching
- regularization
- . . .

Regularization

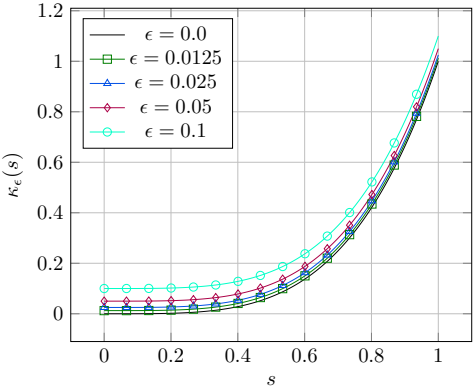


Brooks–Corey **regularized** pressure–saturation functions

Regularization

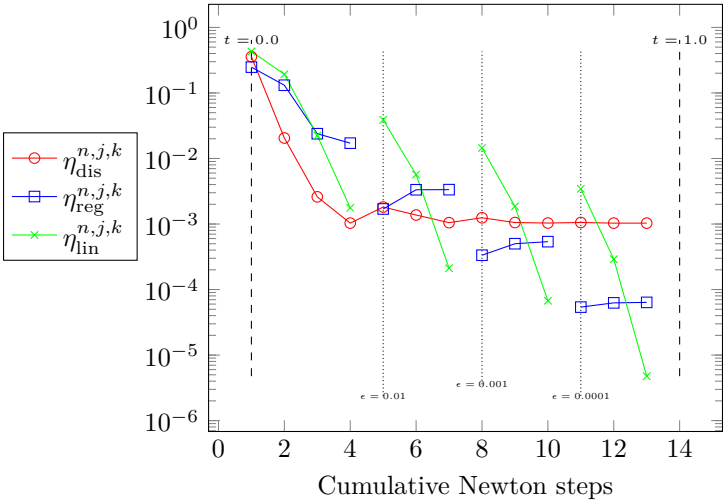


Brooks–Corey **regularized** pressure–saturation functions



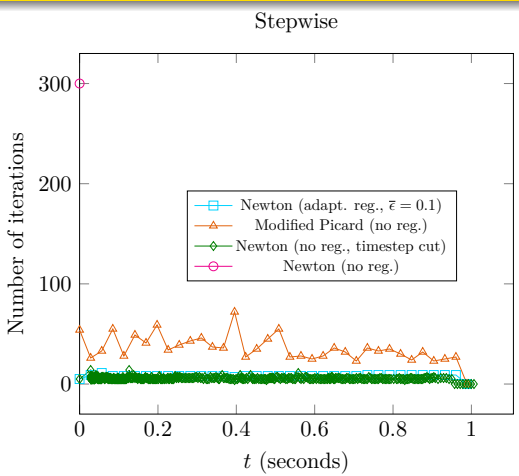
Brooks–Corey **regularized** saturation–relative permeability functions

Example overall behavior (Richards equation, 1 time step)



F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

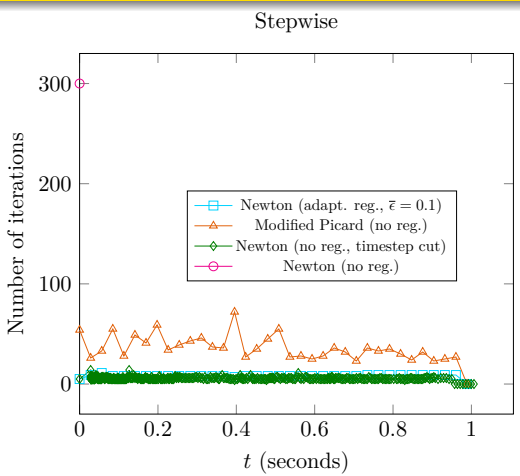
Comparison with existing approaches



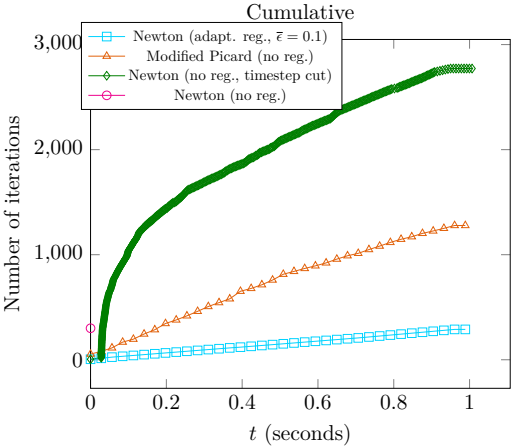
Number of linearization iterations on each time step

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)

Comparison with existing approaches



Number of linearization iterations on each time step



Cumulative number of linearization iterations

F. Févotte, A. Rappaport, M. Vohralík, Computational Geosciences (2024)