A posteriorní odhady chyb a adaptivita v numerických aproximacích parciálních diferenciálních rovnic

Martin Vohralík

Inria Paříž & Ecole des Ponts ParisTech

Brno, 30. listopadu 2021

Outline

1. Research and education in France, Inria, the SERENA research team
2. Introduction: numerical approximation of partial differential equations
3. A posteriori error estimates, balancing of error components, and adaptivity
   - A posteriori error estimates
   - Mesh adaptivity
   - Polynomial-degree adaptivity
   - Balancing of error components (inexact linear and nonlinear solvers)
4. Application to unsteady multi-phase multi-compositional Darcy flow
5. Conclusions

CNRS

National Centre for Scientific Research

- fundamental research
- Institutes of Chemistry, Ecology and Environment, Physics, Nuclear and Particle Physics, Biological Sciences, Humanities and Social Sciences, Computer Sciences, Engineering and Systems Sciences, Mathematical Sciences, Earth Sciences and Astronomy
- 25.500 permanent employees
  - research directors (directeurs de recherche, equivalent to full professor)
  - research scientists (chargés de recherche, equivalent to associate professor)
  - engineers, technicians
  - administrative staff
- 7.500 temporary workers (Ph.D. students, post-docs, engineers, interns)
- researchers typically integrated into university laboratories (few own facilities)
- www.cnrs.fr

Inria

National Institute for Research in Informatics and Automation

- theoretical and applied research in informatics & applied mathematics
- 1.300 research scientists
- 1000 Ph.D. students, 500 post-docs
- 8 research centers in France, 1 in Chile
- organization by project-teams:
  - specific subject
  - 2–10 permanent members
  - often joint with universities
  - 4 years lifespan, evaluation by a international committee, 3 cycles at most
- www.inria.fr

Higher education in France

Public universities

- more than 80 universities
- no entrance examination
- 3-years bachelor, 2-years master

Grandes écoles

- highly selective admission based on national ranking in competitive written and oral exams
- 2 years of dedicated preparatory classes for the exams
- small number of students
- typically a 3-year engineering cycle
- often economy/management/law courses also for engineers

Private universities

- a few smaller institutions

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Ecole Nationale des Ponts et Chaussées

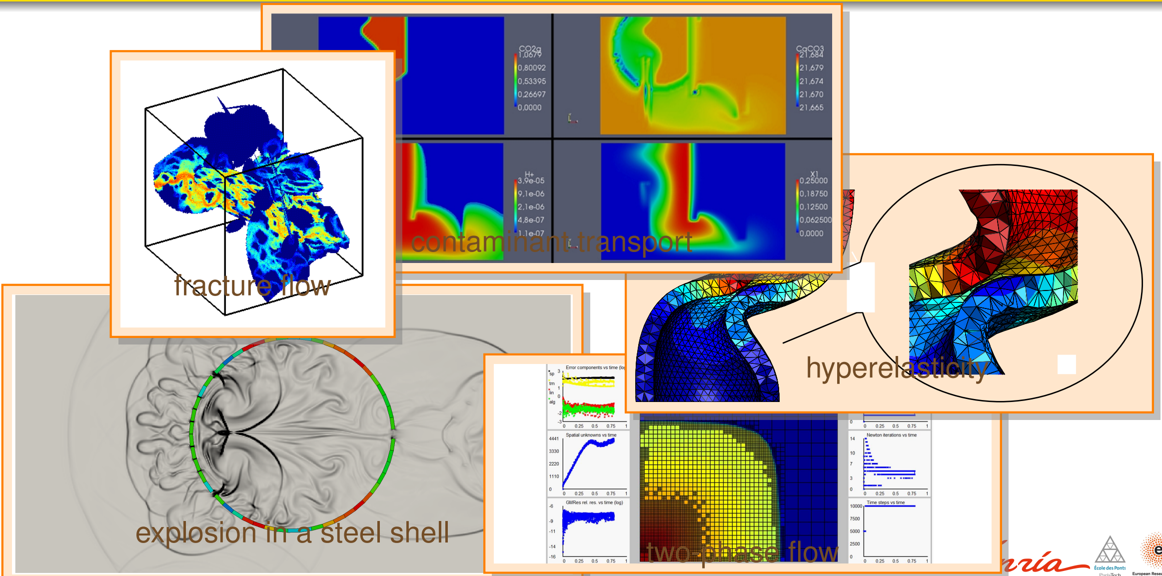
- *Grande école* founded in 1747: build bridges & roads
- highly selective admission based on national ranking in competitive written and oral exams
- 380 research scientists & professors
- small number of students
- famous professors: Navier, Coriolis, d'Ocagne, Séjourné, . . .
- famous students: Bienvenüe, Freyssinet, Caquot, Saint-Venant, Becquerel, Biot, Chauchy, Fresnel, Darcy
- http://www.enpc.fr/en

Project-team SERENA

Simulation for the Environment: Reliable and Efficient Numerical Algorithms

- conception and analysis of models based on partial differential equations (PDEs)
- 6 permanent members, 2 post-docs, 7 Ph.D. students, 1 research engineer
- **numerical** approximation methods (**algorithms**) (finite element method)
- algebraic solvers (domain decomposition, multigrid, Newton–Krylov)
- implementation issues (correctness of programs)
- **reliability** of the overall **simulation**
- **efficiency** with respect to computational resources
- current **environmental** problems
- https://team.inria.fr/serena/

Examples: numerical simulations of PDEs in SERENA



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Partial differential equations (PDEs)

- **describe** numerous **physical phenomena**
  - fluid flow and transport in the underground, air, oceans, rivers (weather forecast, modeling pollution, . . .)
  - solid structure and its deformations (construction of buildings/cars/planes. . .)
  - population dynamics, behavior of financial markets (demography, economy . . .)
  - . . .
- include (partial) derivatives of the solution
- it is almost **never possible** to **find** analytical, **exact solutions**

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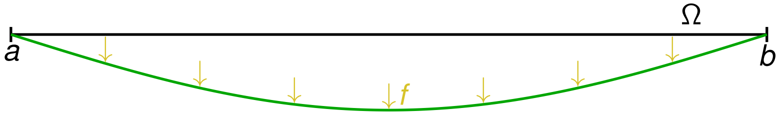
- it is almost **never possible** to **find** analytical, **exact solutions** (not even Einstein could solve PDEs with paper and pen, except in model cases . . .)

Example: elastic string



Elastic string subject to force f:

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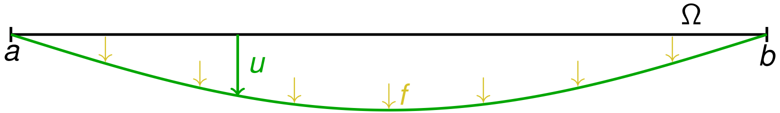

Elastic string subject to force f: displacement u

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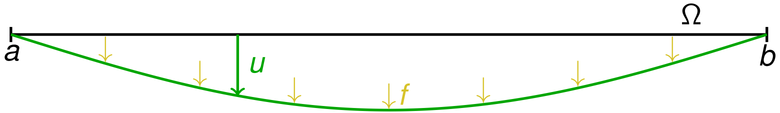

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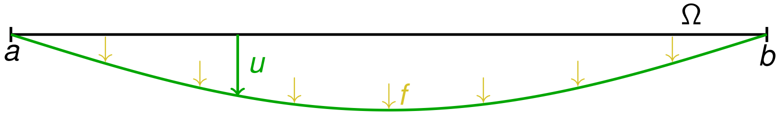

Elastic string subject to force f: displacement u

Let Ω be an interval, $\Omega =]a, b[$, a, b two real numbers, $a < b$. Let $f :]a, b[\to \mathbb{R}$ be a given function. Find $u :]a, b[\to \mathbb{R}$ such that

$$-(u')' = f,$$
$$u(a) = u(b) = 0.$$

Numerical approximations of PDEs

Numerical methods

- mathematically-based algorithms evaluated by **computers**
- deliver **approximate solutions**
- conception: more effort $\Rightarrow$ closer to the unknown solution
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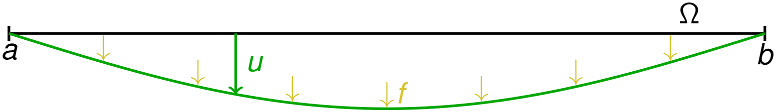

Numerical approximation u_h and its convergence to u

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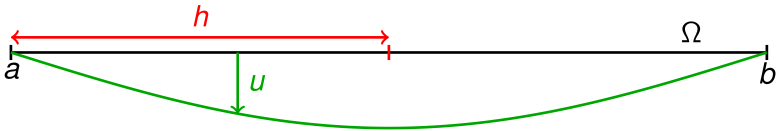

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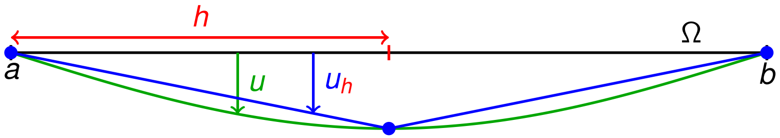

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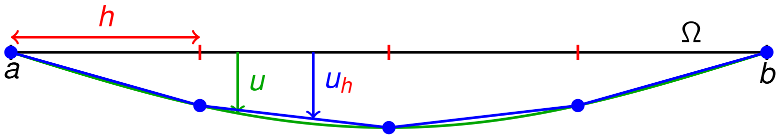

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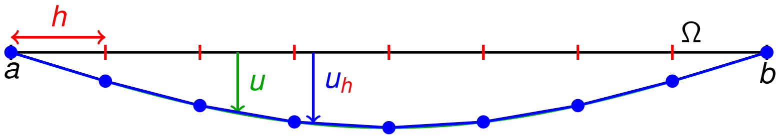

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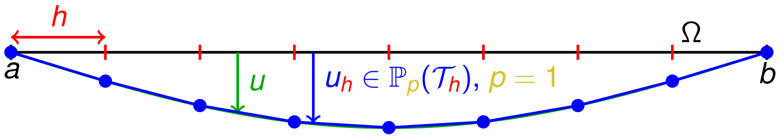

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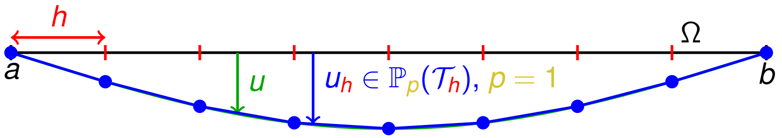

Numerical approximation u_h and its convergence to u

Error

$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

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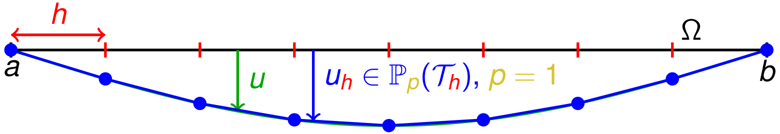

Numerical approximation u_h and its convergence to u

Error

$$\|\nabla(u-u_h)\| = \left\{\int_a^b |(u-u_h)'|^2\right\}^{\frac{1}{2}}$$

Need to solve

$$\mathbb{A}_h \mathrm{U}_h = \mathrm{F}_h$$

3 crucial questions

Crucial questions

1. How **large** is the overall **error**?
2. **Where** (model/space/time/linearization/algebra) is it **localized**?
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Suggested answers

1. **A posteriori** error **estimates**.

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Suggested answers

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

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

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

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ELSEVIER

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

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

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A posteriori error estimates: control the error

Elastic string/membrane equation

$$
\begin{aligned}
-\Delta u &= f \quad \text{in} \quad \Omega,\\
u &= 0 \quad \text{on} \quad \partial\Omega
\end{aligned}
$$

Guaranteed error upper bound (reliability)

$$\underbrace{\|\nabla(u-u_h)\|}_{\text{unknown error}} \qquad \underbrace{\eta(u_h)}_{\text{computable estimator}}$$

Error lower bound (efficiency)

$$\eta(u_h) \le C_{\text{eff}} \|\nabla(u-u_h)\|$$

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How **large** is the overall error? (model pb, known smooth solution)

h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\mathrm{eff}} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
h_0	1	1.25	28%	1.07	24%	1.17
$\approx h_0/2$		[illegible]				
$\approx h_0/4$		[illegible]				
$\approx h_0/8$		[illegible]				
$\approx h_0/2$	2	[illegible]				
$\approx h_0/4$	3	[illegible]				
$\approx h_0/8$	4	[illegible]				

A. Ern, M. Vohralík, SIAM Journal on Numerical Analysis (2015)
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

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$\approx h_0/2$		6.07×10^{-1}	14%	5.56×10^{-1}		
$\approx h_0/4$		3.10×10^{-1}	7.0%	2.92×10^{-1}		
$\approx h_0/8$		1.45×10^{-1}	3.3%	1.39×10^{-1}		
$\approx h_0/2$	2	4.23×10^{-2}	9.5×10^{-1}%	4.07×10^{-2}		
$\approx h_0/4$	3	2.62×10^{-4}	5.9×10^{-3}%	2.60×10^{-4}		
$\approx h_0/8$	4	2.60×10^{-7}	5.9×10^{-6}%	2.58×10^{-7}		

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h	p	$\eta(u_h)$	rel. error estimate $\frac{\eta(u_h)}{\|\nabla u_h\|}$	$\|\nabla(u-u_h)\|$	rel. error $\frac{\|\nabla(u-u_h)\|}{\|\nabla u_h\|}$	$I^{\rm eff} = \frac{\eta(u_h)}{\|\nabla(u-u_h)\|}$
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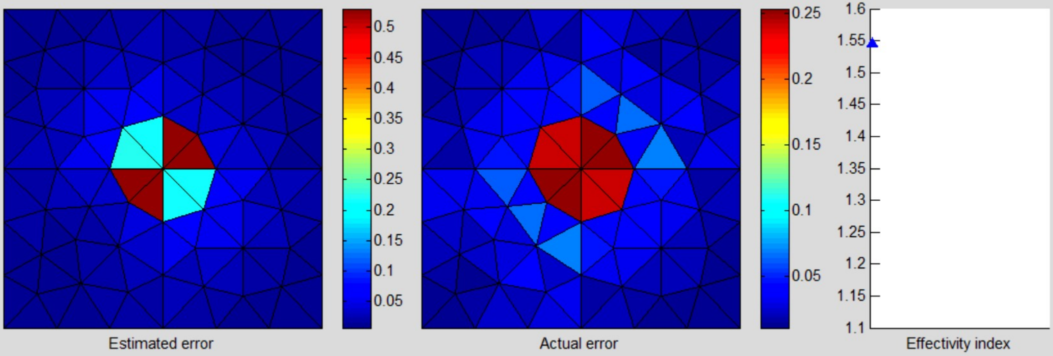
V. Dolejší, A. Ern, M. Vohralík, SIAM Journal on Scientific Computing (2016)

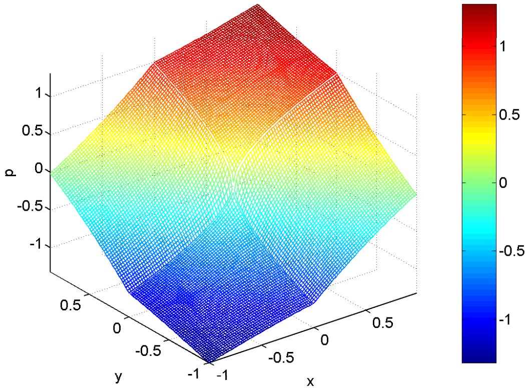
Outline

Adaptive mesh refinement (singular solution)

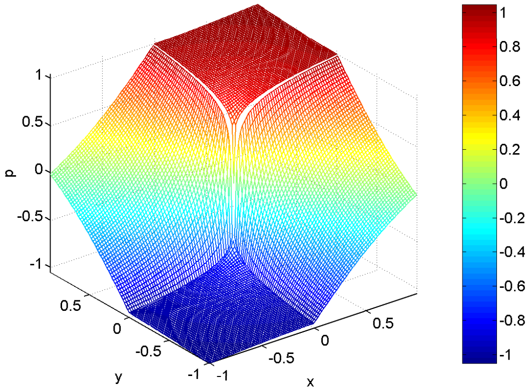


M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Singular solutions

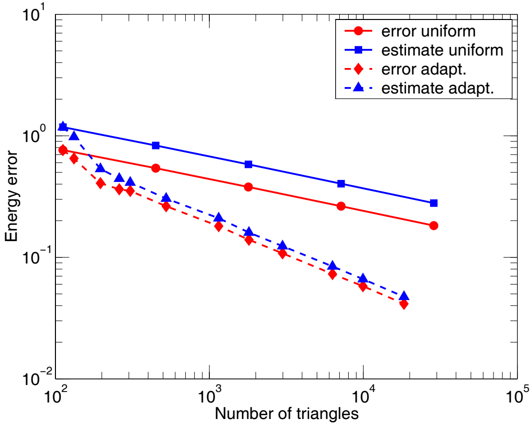


$H^{1.54}$ singularity



$H^{1.13}$ singularity

Estimated and actual error against the number of elements in uniformly/adaptively refined meshes (singular solutions)



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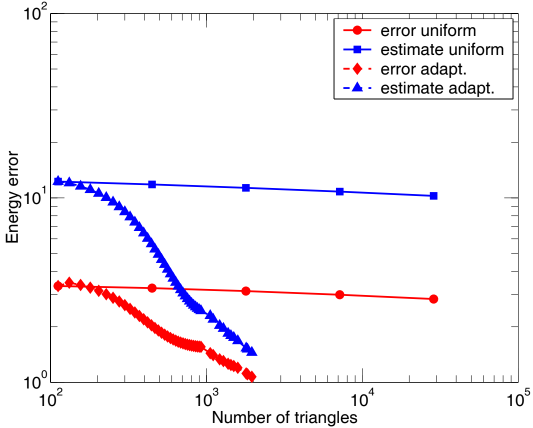

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M. Vohralík, SIAM Journal on Numerical Analysis (2007)

Adaptive mesh refinement

Adaptive mesh refinement

- Dörfler marking: subset $\mathcal{M}_\ell$ containing θ-fraction of the estimates

$$\sum_{K\in\mathcal{M}_\ell} \eta_K(u_\ell)^2 \geq \theta^2 \sum_{K\in\mathcal{T}_\ell} \eta_K(u_\ell)^2$$

Convergence on a sequence of adaptively refined meshes

- $$\|\nabla(u-u_\ell)\| \to 0$$
- some mesh elements may not be refined at all: ~~$h \searrow 0$~~
- Babuška & Miller (1987), Dörfler (1996)

Optimal error decay rate wrt degrees of freedom

- $$\|\nabla(u-u_\ell)\| \lesssim |\mathrm{DoF}_\ell|^{-p/d}$$ (replaces h^p)
- same for smooth & singular solutions: ~~higher-order only pay-off for sm. sol.~~
- decays to zero as fast as on a best-possible sequence of meshes
- Morin, Nochetto, Siebert (2000), Stevenson (2005, 2007), Cascón, Kreuzer, Nochetto, Siebert (2008), Canuto, Nochetto, Stevenson, Verani (2017)

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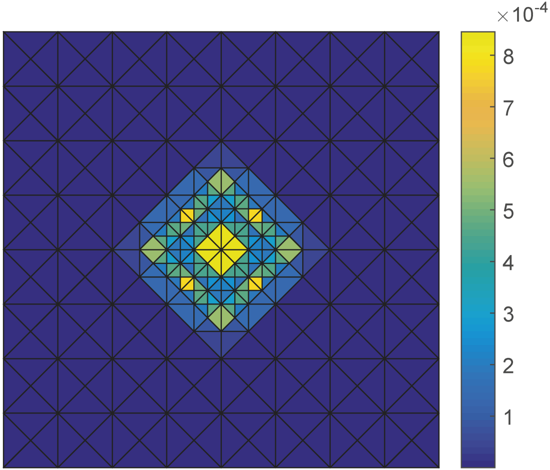
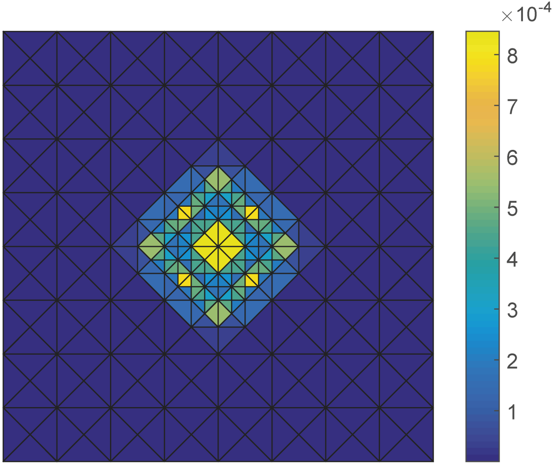
Outline

1. Research and education in France, Inria, the SERENA research team
2. Introduction: numerical approximation of partial differential equations
3. A posteriori error estimates, balancing of error components, and adaptivity
   - A posteriori error estimates
   - Mesh adaptivity
   - Polynomial-degree adaptivity
   - Balancing of error components (inexact linear and nonlinear solvers)
4. Application to unsteady multi-phase multi-compositional Darcy flow
5. Conclusions

Where (in space) is the error **localized**? (known smooth solution)



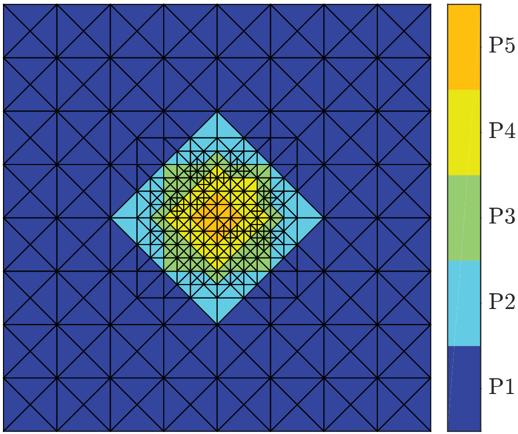
Estimated error distribution $\eta_K(u_h)$



Exact error distribution $\|\nabla(u - u_h)\|_K$

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Best-possible error decrease: *hp* **adaptivity**, (**smooth** solution)



Mesh $\mathcal{T}_\ell$ and pol. degrees p_K

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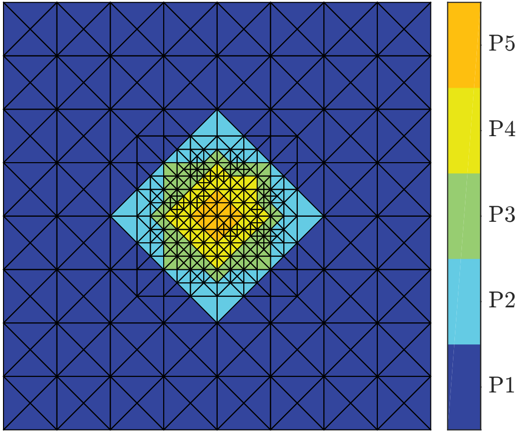

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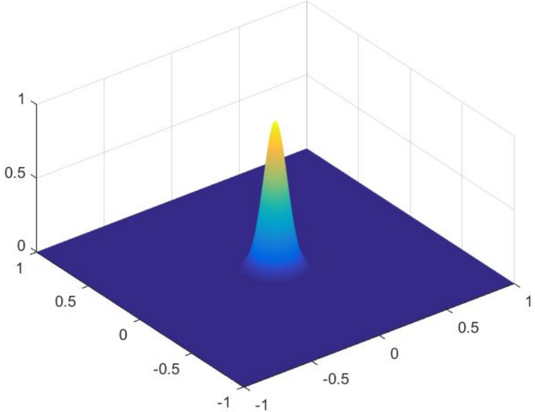

Exact solution

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

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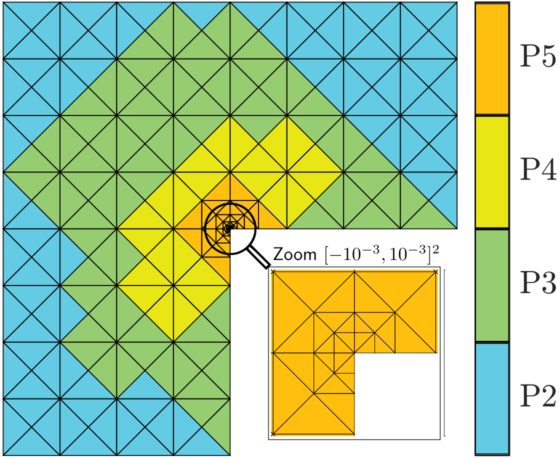

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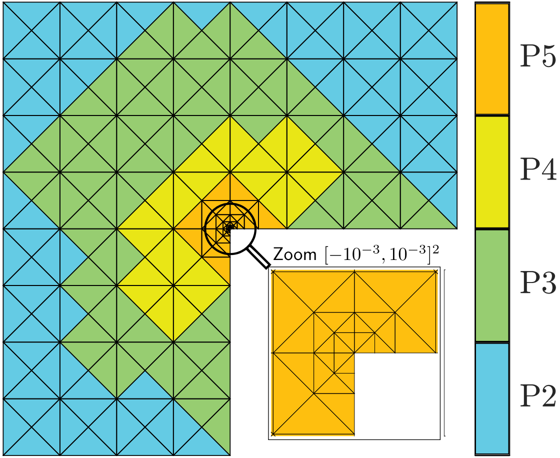

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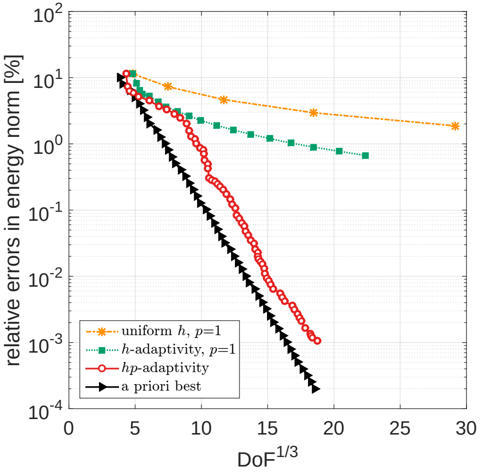

Relative error as a function of DoF

P. Daniel, A. Ern, I. Smears, M. Vohralík, Computers & Mathematics with Applications (2018)

Outline

Balancing error components (nonlinear problem, inexact solvers)

Fully adaptive algorithm (adaptive inexact Newton method)

- **total error estimate** on mesh $\mathcal{T}_\ell$, linearization step k, algebraic solver step i

$$\underbrace{\| u - u_\ell^{k,i} \|_*}_{\text{total error}} \le \underbrace{\eta_{\ell,\mathrm{disc}}^{k,i}}_{\text{discretization estimate}} + \underbrace{\eta_{\ell,\mathrm{lin}}^{k,i}}_{\text{linearization estimate}} + \underbrace{\eta_{\ell,\mathrm{alg}}^{k,i}}_{\text{algebraic estimate}}$$

- **balancing error components**: work where needed

$\eta_{\ell,\mathrm{alg}}^{k,i} \le \gamma_{\mathrm{alg}} \max\{\eta_{\ell,\mathrm{disc}}^{k,i}, \eta_{\ell,\mathrm{lin}}^{k,i}\}$	stopping criterion linear solver
$\eta_{\ell,\mathrm{lin}}^{k,i} \le \gamma_{\mathrm{lin}} \eta_{\mathrm{disc}}^{k,i}$	stopping criterion nonlinear solver
$\theta \eta_{\ell,\mathrm{disc}}^{k,i} \le \eta_{\mathrm{disc},\mathcal{M}_\ell}^{k,i}$	adaptive mesh refinement

- link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuflhard (1991), Eisenstat & Walker (1994)

Convergence, optimal **error decay rate** wrt **DoFs**

- Gantner, Haberl, Praetorius, & Stiftner (2018), Heid & Wihler (2019)

Optimal error decay rate wrt overall computational cost

- Haberl, Praetorius, Schimanko, & Vohralík (2021)

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$$\underbrace{\|u - u_\ell^{k,i}\|_*}_{\text{total error}} \le \underbrace{\eta^{k,i}_{\ell,\mathrm{disc}}}_{\text{discretization estimate}} + \underbrace{\eta^{k,i}_{\ell,\mathrm{lin}}}_{\text{linearization estimate}} + \underbrace{\eta^{k,i}_{\ell,\mathrm{alg}}}_{\text{algebraic estimate}}$$

- **balancing error components**: work where needed

$\eta^{k,i}_{\ell,\mathrm{alg}} \le \gamma_{\mathrm{alg}} \max\{\eta^{k,i}_{\ell,\mathrm{disc}}, \eta^{k,i}_{\ell,\mathrm{lin}}\}$	stopping criterion linear solver,
$\eta^{k,i}_{\ell,\mathrm{lin}} \le \gamma_{\mathrm{lin}} \eta^{k,i}_{\mathrm{disc}}$	stopping criterion nonlinear solver,
$\theta\eta^{k,i}_{\ell,\mathrm{disc}} \le \eta^{k,i}_{\mathrm{disc},\mathcal{M}_\ell}$	adaptive mesh refinement

- link – inexact Newton method: Bank & Rose (1982), Hackbusch & Reusken (1989), Deuflhard (1991), Eisenstat & Walker (1994)

Convergence, optimal **error decay rate** wrt **DoFs**

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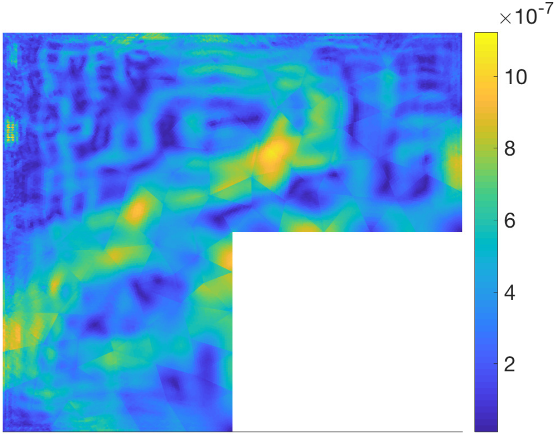
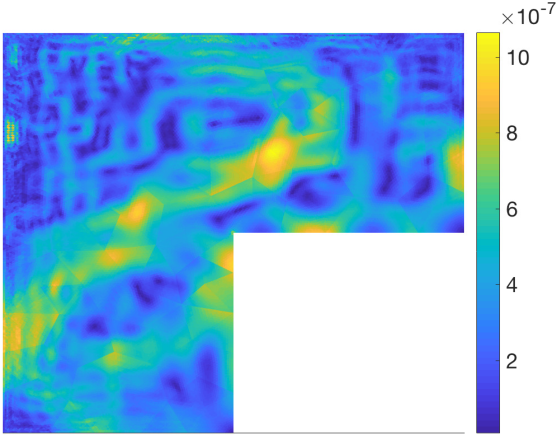
Including **algebraic error**: $\mathbb{A}_\ell \mathsf{U}_\ell^i \neq \mathsf{F}_\ell$



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)

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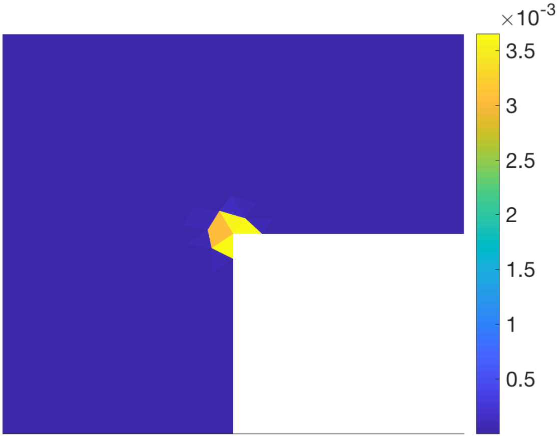
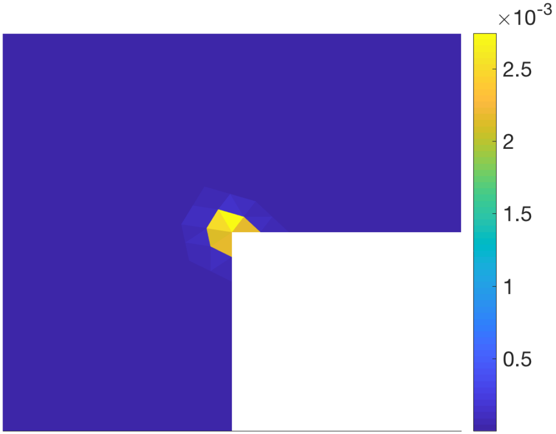


Estimated total errors $\eta_K(u_\ell^i)$



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)

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

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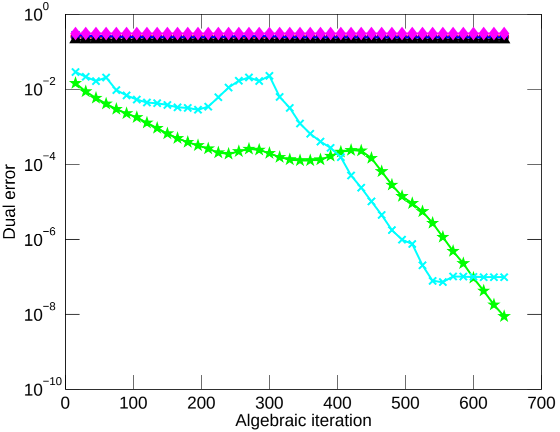

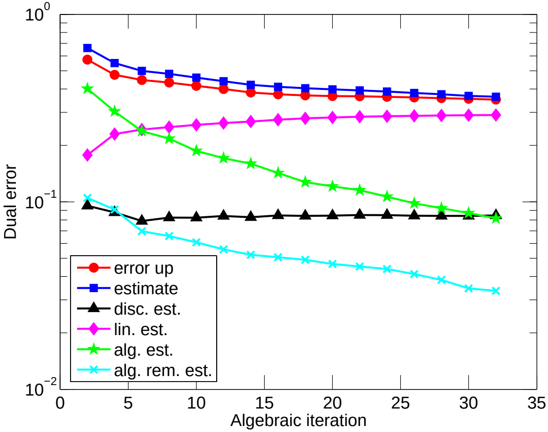

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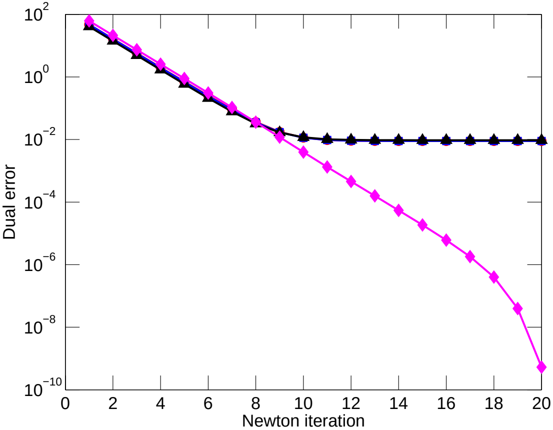

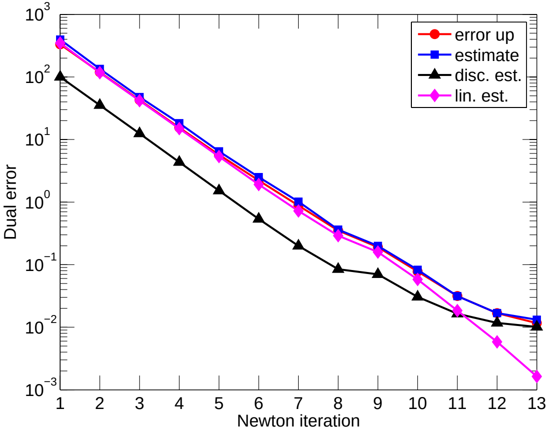

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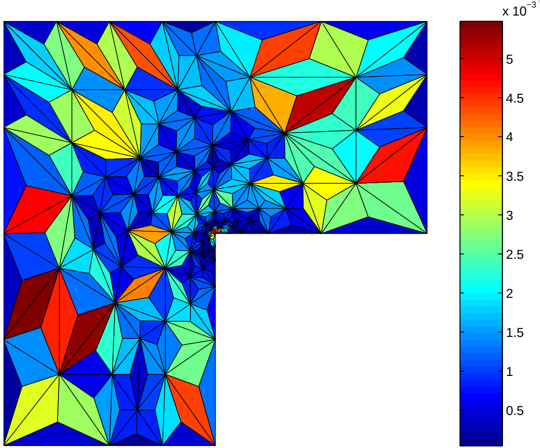

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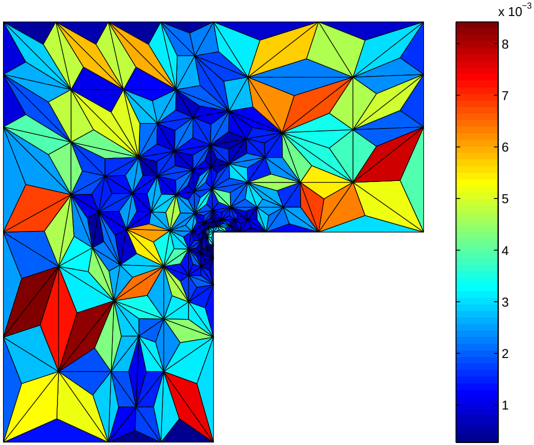
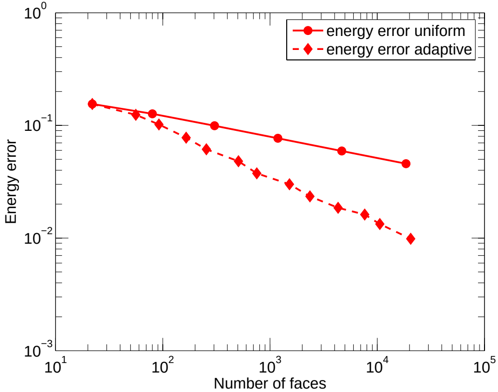


Exact errors $\|\boldsymbol{\sigma}(\nabla u) - \boldsymbol{\sigma}(\nabla u_\ell^{k,i})\|_{q,K}$

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

Convergence and optimal decay rate wrt DoFs/computational cost



Optimal decay rate wrt DoFs

classical		
	alg. solver iter last mesh	550
	relative error estimate	4.6%

adaptive		
	alg. solver iter last mesh	242
	relative error estimate	1.1%

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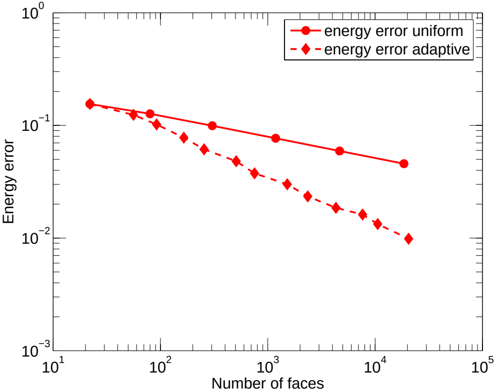

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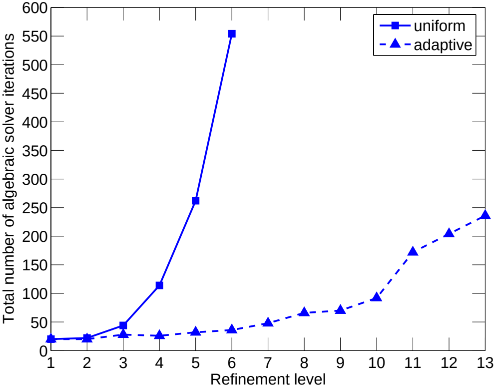

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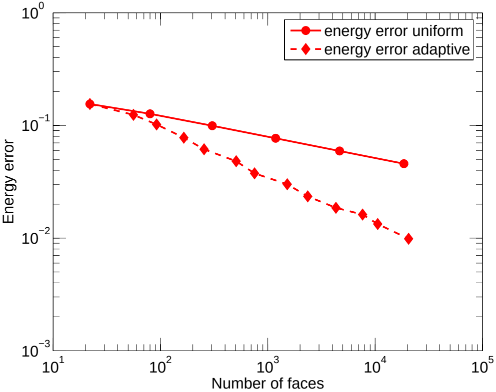

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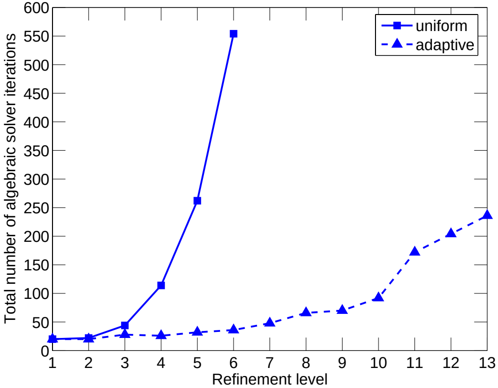

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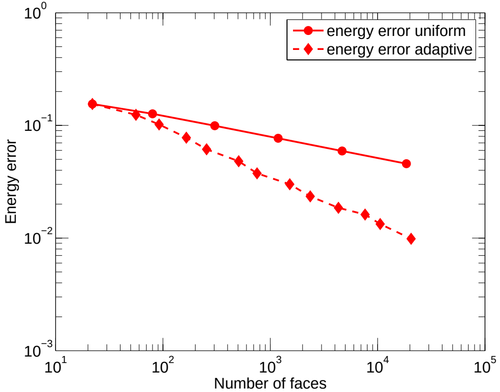

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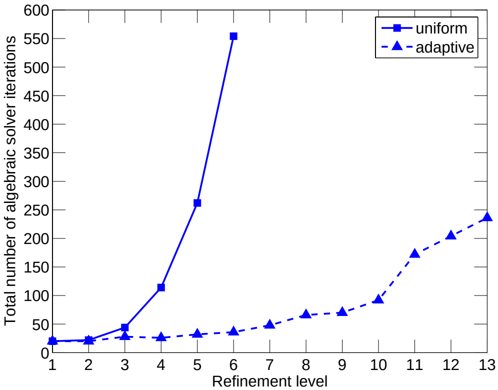

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Outline

Realistic environmental problem

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

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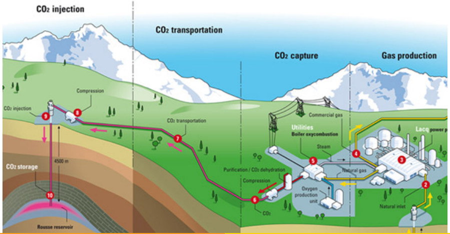
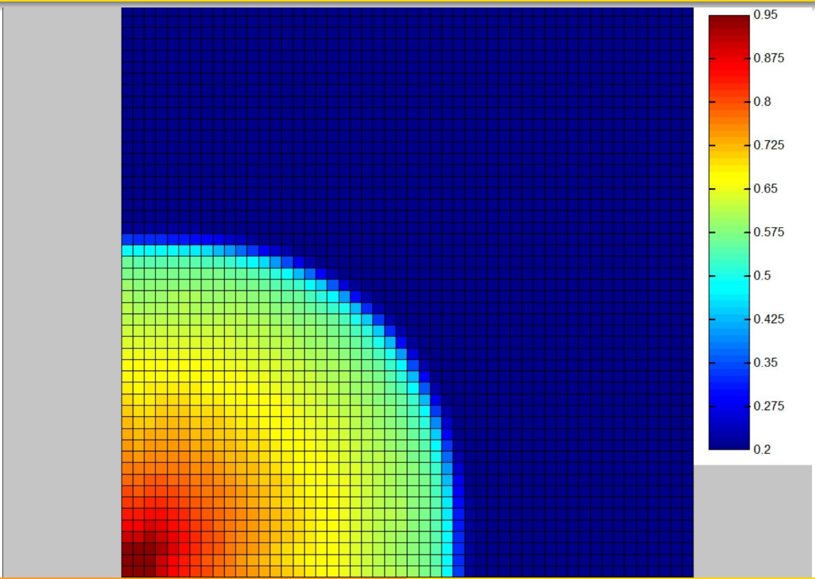
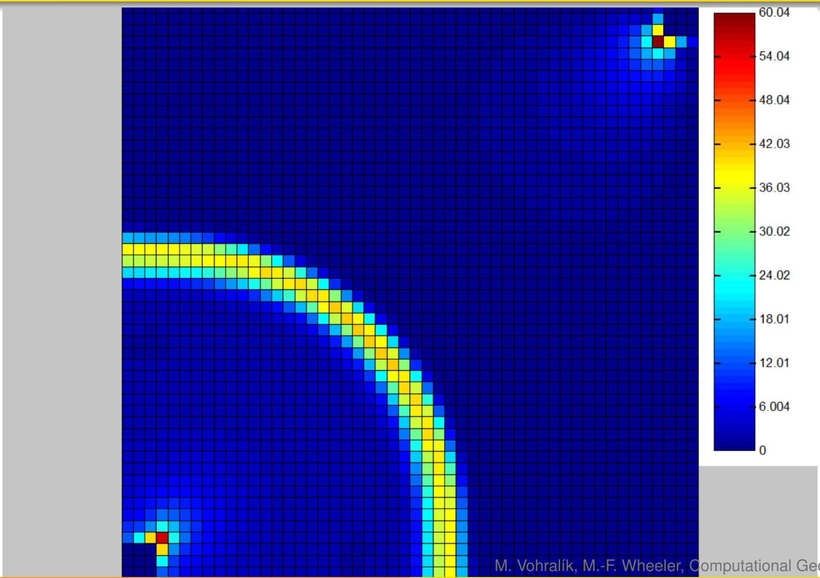
Carbon capture & geological storage



Water saturation evolution

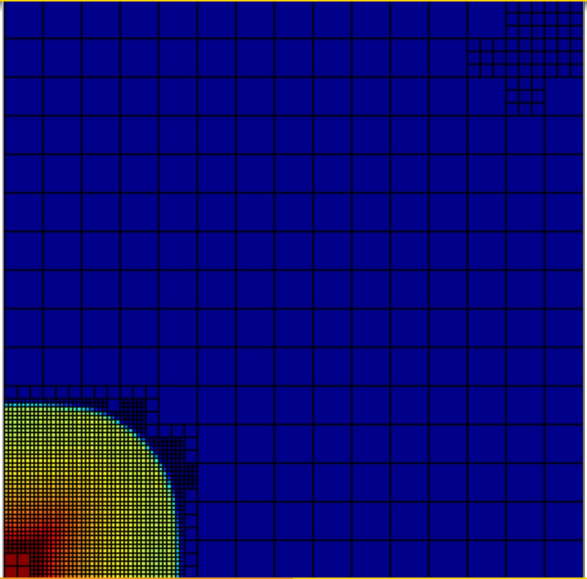


A posteriori error estimate



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

Space/time/nonlinear solver/linear solver adaptivity



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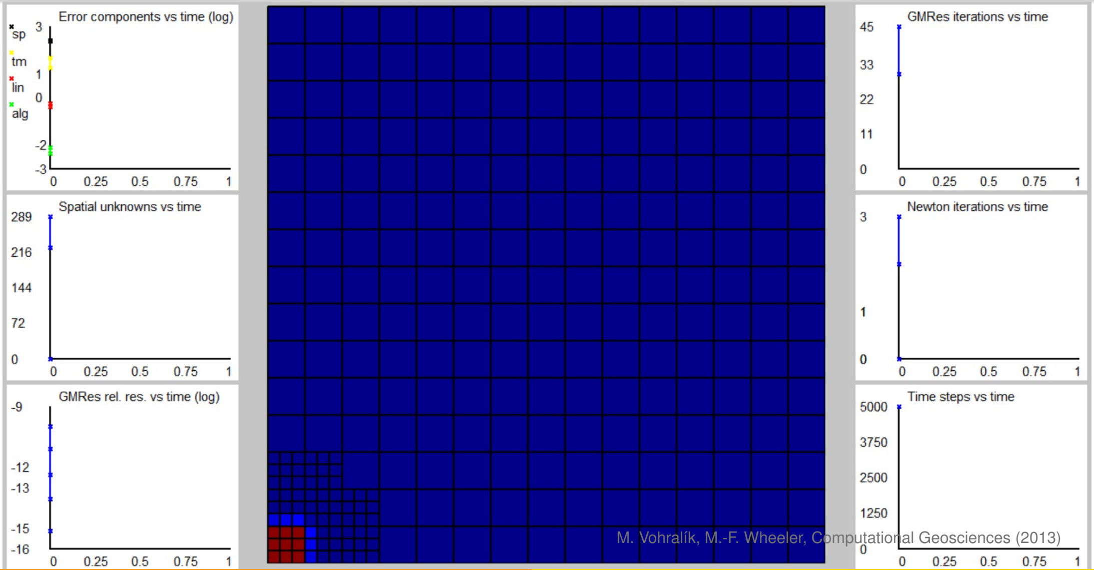

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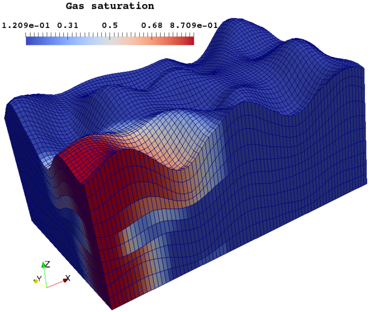
Black-oil multiphase problem (collaboration IFPEN)



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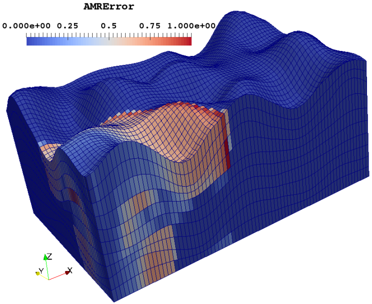

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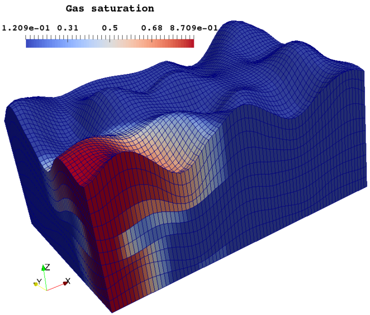

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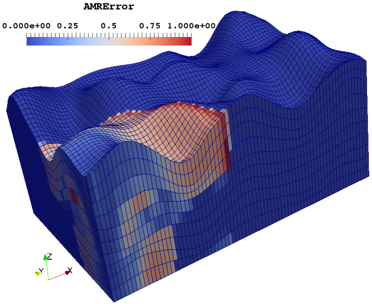

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A posteriori estimates

1. **certify the error**
2. **localize** it in space & time
3. **distinguish** its **components**
4. **decrease** it **efficiently** via **adaptivity**

Outline

1. Research and education in France, Inria, the SERENA research team
2. Introduction: numerical approximation of partial differential equations
3. A posteriori error estimates, balancing of error components, and adaptivity
   - A posteriori error estimates
   - Mesh adaptivity
   - Polynomial-degree adaptivity
   - Balancing of error components (inexact linear and nonlinear solvers)
4. Application to unsteady multi-phase multi-compositional Darcy flow
5. Conclusions

Conclusions

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- a posteriori **error control**
- **full adaptivity**: linear solver, nonlinear solver, time step, space mesh, polynomial degree
- recovering **mass balance** in any situation

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VOHRALÍK M., A posteriori error estimates for lowest-order mixed finite element discretizations of convection-diffusion-reaction equations, *SIAM J. Numer. Anal.* **45** (2007), 1570–1599.

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.

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., YOUSEF S., A simple a posteriori estimate on general polytopal meshes with applications to complex porous media flows, *Comput. Methods Appl. Mech. Engrg.* **331** (2018), 728–760.

Thank you for your attention!

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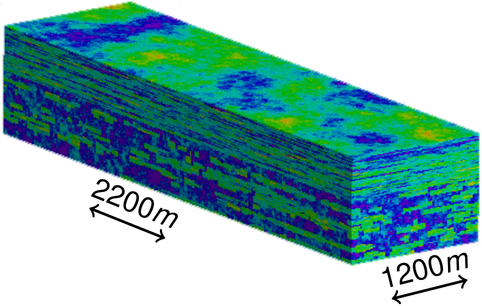
Thank you for your attention!

Error in a quantity of interest (goal functional) (certify error in practice): $-\nabla\cdot(\mathbf{K}\nabla u) = f$: outflow error $\left|\int_{y=2200} \mathbf{K}\nabla(u-u_\ell)\cdot\mathbf{n}\right|$

no of unknowns	825	3300	13200
rel. error est.	46%	34%	24%



Underground reservoir,
10th SPE test case

G. Mallik, M. Vohralík, S. Yousef, Journal of Computational and Applied Mathematics (2019)

Error in a quantity of interest (goal functional) (certify error in practice): $-\nabla\cdot(\mathbf{K}\nabla u) = f$: outflow error $\left|\int_{y=2200} \mathbf{K}\nabla(u-u_\ell)\cdot\mathbf{n}\right|$

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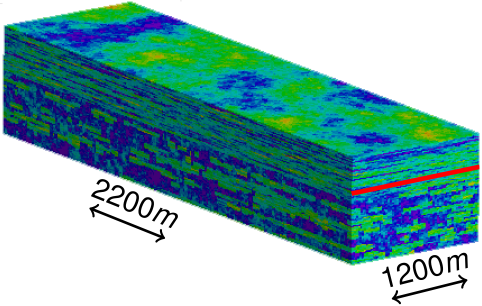

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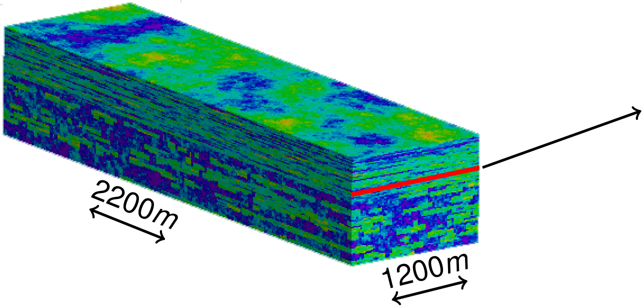

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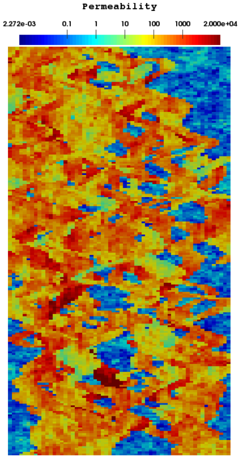

Layer permeability

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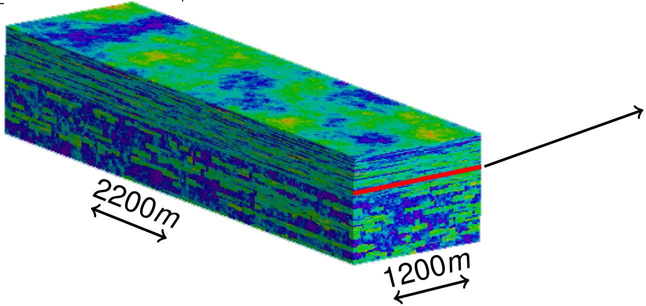

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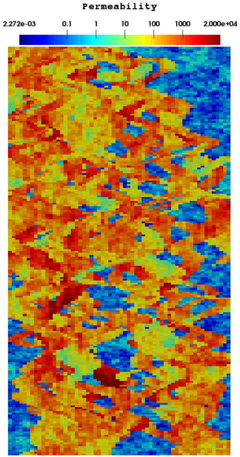

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